MAMT

93-018

The Critical Temperature and Gap Solution in the Bardeen-Cooper-Schrieffer Theory of Superconductivity

Q.Du
Carnegie Mellon University
Y. Yang
Carnegie Mellon University

Research Report No. 93-NA-018

May 1993

Sponsors

U.S. Army Research Office
Research Triangle Park
NC 27709

National Science Foundation
1800 G Street, N.W.
Washington, DC 20550

NAMT

93-018

The Critical Temperature and Gap Solution in the Bardeen–Cooper–Schrieffer Theory of Superconductivity

QIANG DU* & YISONG YANG†

Abstract

The paper studies the problem of numerical approximations of the critical transition temperature and the energy gap function in the Bardeen–Cooper–Schrieffer equation arising in superconductivity theory. The positive kernel function leads to a phonon dominant state at zero temperature. Much attention is given to the equation defined on a bounded region. Two discretized versions of the equation will be introduced. The first version approximates the desired solution from below, while the second, from above. Numerical examples are presented to illustrate the efficiency of the method. Besides, The approximations of a full space solution and the associated critical temperature by solution sequences constructed on bounded domains are also investigated.

AMS subject classifications (1991). 82B26, 82D55, 45G10, 45L.

1 Introduction

In the Bardeen–Cooper–Schrieffer (BCS) quantum theory of superconductivity, the superconducting state is characterized by a positive gap function, $\Delta(\mathrm{k})$ (say), which is the solution of the BCS equation (see, for example, [H] and [vH])

$$\Delta(\mathrm{k}) = \int \mathrm{dk}' K(\mathrm{k},\mathrm{k}')\varphi_\beta(\mathrm{k}',\Delta(\mathrm{k}')), \tag{1.1}$$

where

$$\varphi_\beta(\mathrm{k}',\Delta(\mathrm{k}')) = H_\beta(([\mathrm{k}'^2-\mu]^2+\Delta^2(\mathrm{k}'))^{1/2})\Delta(\mathrm{k}') \tag{1.2}$$

*Department of Mathematics, Michigan State University, East Lansing, MI 48824. Part of this work was done while this author was visiting the department of mathematics, Carnegie Mellon University, Pittsburgh, PA 15213.

†Department of Mathematics, Carnegie Mellon University, Pittsburgh, PA 15213.

with

$$H_\beta(t) = \frac{\tanh(\frac{1}{2}\beta t)}{t}, \tag{1.3}$$

$\mu > 0$ being the chemical potential or Fermi energy, β the inverse of the absolute temperature, $T \geq 0$, $K(\mathbf{k}, \mathbf{k}') = -V_{\mathbf{k}\mathbf{k}'}$ the negative matrix elements of the interaction potential of electrons with wave vectors $\mathbf{k}, \mathbf{k}' \in \mathbf{R}^3$, and $\mathbf{k}^2 = |\mathbf{k}|^2$. In general, $V_{\mathbf{k}\mathbf{k}'}$ is the sum of two terms. The first term, positive, arises from the repulsive Coulomb force, while the second one, negative, from the attractive phonon force. For a superconductor, the basic BCS assumption says that $V_{\mathbf{k}\mathbf{k}'} < 0$ (or $K(\mathbf{k}, \mathbf{k}') > 0$), namely, the dominance of phonon interaction is assumed. In this situation, electrons can form Cooper pairs at low temperatures, or equivalently, the equation (1.1) now has a bounded positive solution (the energy gap), which leads to the birth of supercurrent. As a consequence, superconductivity takes place. Such a global phase transition picture was already known to BCS under the over-simplified condition

$$V_{\mathbf{k}\mathbf{k}'} = \begin{cases} -V_0, \quad V_0 > 0, & |\mathbf{k}|, |\mathbf{k}'| \leq r_0, \\ 0, & |\mathbf{k}|, |\mathbf{k}'| > r_0. \end{cases} \tag{1.4}$$

Here $r_0^2 > \mu$. The recent work [Y] shows that, when $V_{\mathbf{k}\mathbf{k}'}$ is a negative continuous function, the above phase transition still holds in general. More precisely, it has been proved there that, if

$$K(\mathbf{k}, \mathbf{k}') \leq \sigma(\mathbf{k}'), \qquad \frac{\sigma(\mathbf{k})}{\mathbf{k}^2 + 1} \in L(\mathbf{R}^3) \tag{1.5}$$

(to ensure boundedness of solutions), then there is a critical temperature $T_c > 0$, so that, for $0 \leq T = 1/\beta < 1/\beta_c = T_c$, the BCS equation (1.1) on $\mathbf{R}^3$ has a positive gap solution $\Delta(\mathbf{k}) > 0$, representing the occurrence of superconductivity, while for $T = 1/\beta > 1/\beta_c = T_c$, the only solution of (1.1) is the trivial one, $\Delta(\mathbf{k}) \equiv 0$, indicating the dominance of the normal phase.

The next important problem is to determine numerically the critical temperature T_c and the gap function $\Delta(\mathbf{k})$ for $T < T_c$. The resolution of this problem is of obvious practical value. However, due to the complexity of (1.1), there have only been credible computations of (1.1) for the over-simplified kernel function (1.4) or for equations with separable kernels in literature, although early in [K] the convergence of an iterative procedure is studied at the zero temperature limit. The main purpose of this paper is to provide a reliable numerical method to compute both the solution and the critical temperature of (1.1) on an arbitrary bounded region. The approximation of a solution in full $\mathbf{R}^3$ by solutions sequences on bounded regions will also be investigated under some conditions.

The paper is organized as follows. In Section 2 we introduce two discretized versions of (1.1) on a bounded region, called the min-min and the max-max approximations. We show that these approximations lead to two critical temperatures, τ_c' and τ_c'', respectively, and $\tau_c' \leq T_c \leq \tau_c''$, where T_c is the critical temperature of (1.1) on the given bounded region. Below the critical temperatures, the discretized BCS equations have positive solutions, Δ' and Δ'' with $\Delta' \leq \Delta \leq \Delta''$, where Δ is the unique positive solution of (1.1). We will point out that finer discretizations yield better approximations. In Section 3 we study the connection between full space solutions and solutions obtained on bounded regions. We shall also show that the uniqueness of a full space solution there follows naturally as a by-product. In Section 4 we discuss in detail a series of numerical solutions constructed from the method of this paper. We choose a radially symmetric limit to study and the discretizations can be viewed as being made by a sequence of spherical shells contained in a ball. Monotone convergence, approximation of the critical temperature from below and above, dependence of the number of iterations on the range of the temperature parameter, and so on, are discussed. These examples confirm very well our theoretical expectations.

Note that, in some circumstances, especially in the theoretical developments of high-T_c superconductivity theory [D, E], the kernel function $K(\mathbf{k},\mathbf{k}')$ in (1.1) may be allowed to change signs or be a complex function with a correspondingly modified nonlinear self-coupling φ_β. See e.g. [WE, WEH]. For these models, our method does not apply. However, it is our hope that the study here may serve as an initial step toward a better understanding of the BCS type equations.

2 The Method of Approximation

In this section, the BCS equation (1.1) is assumed to be defined on a bounded region Ω containing the ball

$$\{\mathbf{k} \in \mathbf{R}^3 \,|\, \mathbf{k}^2 \leq 2\mu\}$$

(say) and the kernel $K(\mathbf{k},\mathbf{k}')$ is continuous on $\overline{\Omega}$ and non-negative (for greater generality). The basic positivity condition imposed in this section takes the form

$$K(\mathbf{k},\mathbf{k}') > 0 \quad \text{in } \overline{O}_{\mu,\delta} \times \overline{O}_{\mu,\delta}, \qquad O_{\mu,\delta} = \{\mathbf{k} \in \mathbf{R}^3 \,|\, |\mathbf{k}^2 - \mu| < \delta\}, \tag{2.1}$$

where $\delta > 0$ is small.

To discretize (1.1), we introduce a partition of Ω as follows. Let $\{\Omega_j \,|\, 1 \leq j \leq n\}$

be a collection of open subsets of Ω such that

$$\Omega_j \cap \Omega_k = \emptyset \ (j \neq k), \qquad \cup_{j=1}^{n} \overline{\Omega}_j \supset \Omega.$$

2.1. The min-min scheme

We first approximate the BCS equation (1.1) over Ω by the following discretized equation

$$\begin{aligned} U &= \{u_j\} \in \mathbf{R}^n, \\ u_j &= (m(U))_j \\ &\equiv \min_{\mathbf{k}\in\overline{\Omega}_j} \sum_{k=1}^{n} \min_{\mathbf{k}'\in\overline{\Omega}_k} K(\mathbf{k},\mathbf{k}')F_\beta(\mathbf{k}',u_k)u_k|\Omega_k|, \end{aligned} \tag{2.2}$$

where $F_\beta(\mathbf{k},u) = H_\beta(([\mathbf{k}^2-\mu]^2+u^2)^{1/2})$ (see (1.2)). We call this scheme the min-min approximation of (1.1).

We say that $U = \{u_j\} \in \mathbf{R}^n$ is positive (non-negative), if $u_j > 0$ ($u_j \geq 0$) for $j = 1, 2, \cdots, n$. We write $U > 0$ ($U \geq 0$). Besides, we say $U > V$ ($U \geq V$) if $U - V > 0$ ($U - V \geq 0$). We use the notation

$$\mathcal{C} = \{U \in \mathbf{R}^n \mid U = \{u_j\},\, u_j \geq 0\}$$

to denote the set of non-negative vectors. In the sequel, we will only be interested in non-negative solutions.

For (2.2), we can state

Theorem 2.1. *There is a suitable partition $\{\Omega_j \,|\, 1 \leq j \leq n\}$ of Ω to ensure the existence of a number $\beta_c' > 0$ so that (2.2) has a nontrivial solution in $\mathcal{C}$ for any $\beta : \beta_c' < \beta \leq \infty$, while for $\beta < \beta_c'$, the only solution of (2.2) is the trivial one, $U = 0$. A positive solution is also unique. If in addition, the kernel function satisfies $K(\mathbf{k},\mathbf{k}') = H(\mathbf{k},\mathbf{k}')h(\mathbf{k}')$ with $H(\mathbf{k},\mathbf{k}') > 0$ on $\overline{\Omega}\times\overline{\Omega}$ and $h(\mathbf{k}') > 0$ on $\partial\Omega$, then a nontrivial solution at any $\beta > \beta_c'$ must be positive and, hence, unique. Besides, at $\beta = \beta_c'$, the only solution of (2.2) in $\mathcal{C}$ is the zero solution.*

The purpose of such a result is to use $1/\beta_c'$ as a lower estimate for the critical temperature in the continuous equation (1.1). We remark that sometimes the existence of β_c' may fail if the partition of Ω is not chosen properly. For example, when a partition is fixed and $K(\mathbf{k},\mathbf{k}')$ is so small that m becomes a contraction in $\mathbf{R}^n$ at $\beta = \infty$, then it is easily checked that m is a contraction at any $\beta > 0$. In other words, there is no β so that (1.1) has a nontrivial solution because $U = 0$ is already a solution.

We split the proof of Theorem 2.1 into several steps.

Lemma 2.2. *$m : \mathbf{R}^n \to \mathbf{R}^n$ is a monotone operator in the cone C in the sense that $m : C \to C$ and $m(U) \le m(V)$ for $U \le V$. Besides, if the additional condition in Theorem 2.1 is valid, then there is partition of Ω so that $m(U) < m(V)$ for $U < V$. Moreover, m is increasing in $\beta > 0$.*

Proof. This is because $F_\beta(\mathbf{k}', u)$ $(u \in \mathbf{R})$ increases in $u \ge 0$ and in $\beta > 0$. □

Lemma 2.3. *When $\beta > 0$ is small, the only solution of (2.1) is the trivial one, $U = 0$.*

Proof. If β is small, the property of F_β (see (1.2)) implies that m is a contraction. So m has only one fixed point in $\mathbf{R}^n$ which is the zero vector. □

Lemma 2.4. *There is a partition $\{\Omega_j \,|\, 1 \le j \le n\}$ of Ω so that when $\beta > 0$ is sufficiently large, the equation (2.1) has a nontrivial subsolution, $\underline{U}$, in C to make $m(\underline{U}) \ge \underline{U}$.*

Proof. Recall (2.1). Let $K(\mathbf{k}, \mathbf{k}') \ge c_0 > 0$ in $\overline{O}_{\mu,\delta} \times \overline{O}_{\mu,\delta}$. Since

$$\begin{aligned} I(\varepsilon) = & \int_{O_{\mu,\delta}} \frac{d\mathbf{k}'}{([\mathbf{k}'^2 - \mu]^2 + \varepsilon^2)^{1/2}} \\ = & \ 4\pi \int_{\sqrt{\mu-\delta}}^{\sqrt{\mu+\delta}} \frac{\rho^2 \, d\rho}{([\rho^2 - \mu]^2 + \varepsilon^2)^{1/2}} \to \infty \quad \text{as } \varepsilon \to 0, \end{aligned}$$

there is an $\varepsilon_0 > 0$ so that $I(\varepsilon_0) \ge 3/c_0$. Hence, if $\beta > 0$ is sufficiently large, there holds

$$\begin{aligned} \int_{O_{\mu,\delta}} F_\beta(\mathbf{k}', \varepsilon_0) \, d\mathbf{k}' = & \int_{O_{\mu,\delta}} \frac{\tanh(\frac{1}{2}\beta([\mathbf{k}'^2 - \mu]^2 + \varepsilon_0^2)^{1/2})}{([\mathbf{k}'^2 - \mu]^2 + \varepsilon_0^2)^{1/2}} \, d\mathbf{k}' \\ \ge & \ \frac{2}{c_0}. \end{aligned}$$

As a consequence, we can find a partition of $O_{\mu,\delta}$, say $\{O_j \,|\, 1 \le j \le n-1\}$, so that

$$\sum_{k=1}^{n-1} \min_{\mathbf{k}' \in \overline{O}_k} F_\beta(\mathbf{k}', \varepsilon_0) |O_k| > \frac{1}{c_0}.$$

Therefore,

$$\min_{\mathbf{k}\in\overline{O}_j}\sum_{k=1}^{n-1}\min_{\mathbf{k}'\in\overline{O}_k} K(\mathbf{k},\mathbf{k}')F_\beta(\mathbf{k}',\varepsilon_0)|O_k| > 1. \tag{2.3}$$

Let Ω_n be the complement of $\overline{O}_{\mu,\delta}$ in Ω and $\Omega_j = O_j$, $j = 1,2,\cdots,n-1$. Then $\{\Omega_j \,|\, 1 \le j \le n\}$ is a partition of Ω. Define $\underline{U} = \{u_j\} \in \mathcal{C} \subset \mathbf{R}^n$ by setting

$$u_j = \varepsilon_0, \quad j = 1,2,\cdots,n-1, \quad u_n = 0.$$

From (2.3) we see that $m(\underline{U}) \ge \underline{U}$ as expected. □

Lemma 2.5. *There is a $\delta_0 > 0$ so that for any $\delta \ge \delta_0$, the vector $\overline{U} = \{u_j\} \in \mathbf{R}^n$ with $u_j = \delta, j = 1,2,\cdots,n$ is a supersolution of (2.2) for any $\beta : 0 < \beta \le \infty$, in the sense that $m(\overline{U}) < \overline{U}$. Moreover, if $\underline{U}$ is a subsolution of (2.2), then $\underline{U} < \overline{U}$.*

Proof. It is obvious that the structure of the function $F_\beta(\mathbf{k}', u)$ allows us to find a number $\delta_0 > 0$ so that for $\delta \ge \delta_0$, there holds

$$\max_{\mathbf{k},\mathbf{k}'\in\overline{\Omega}} K(\mathbf{k},\mathbf{k}')F_\beta(\mathbf{k}',\delta)|\Omega| < 1, \qquad 0 < \beta \le \infty.$$

Define $\overline{U} = \{u_j\} \in \mathbf{R}^n$ by setting $u_j = \delta$, $j = 1,2,\cdots,n$. We have $m(\overline{U}) < \overline{U}$. Namely $\overline{U}$ is a supersolution of (2.2).

Let $\underline{U}$ be a subsolution of (2.2) with $\underline{U} = \{\underline{u}_j\}$. If there is a k $(1 \le k \le n)$ so that

$$\underline{u}_k = \max_{1\le j\le n} \underline{u}_j \ge \delta_0,$$

then $\overline{U} = \{u_j\}$ with $u_j = \underline{u}_k$, $j = 1,2,\cdots,n$, is a supersolution produced above. The monotonicity of m (see Lemma 2.2) says that $u_k \le (m(\underline{U}))_k \le (m(\overline{U}))_k < (\overline{U})_k = \underline{u}_k$, which is a contradiction. □

Lemma 2.6. *If (2.2) has a nontrivial subsolution $\underline{U} \in \mathcal{C}$, then it has a nontrivial solution in $\mathcal{C}$.*

Proof. Let $\overline{U}$ be a supersolution produced in Lemma 2.5. Introduce the iterative sequence

$$U_{\ell+1} = m(U_\ell), \qquad \ell = 1,2,\cdots, \qquad U_1 = \overline{U}.$$

The monotonicity of m and the fact $\underline{U} < \overline{U}$ (Lemma 2.5) imply that

$$\underline{U} < \cdots \le U_\ell \le \cdots \le U_2 \le U_1 = \overline{U}.$$

Hence *U* = lim/^oo *Ut* is a solution of (2.2) satisfying *LL≤U<U.* Q

We can now proceed to prove Theorem 2.1.

Set

A s= {/? | *fi* > 0 is such that (2.2) has a nontrivial solution in *C}.*

We claim that A is an interval. To see this, we need only to show that if *fa* < /?2, *fa* G A, then *fa* G A. In fact, if we denote by *U* a nontrivial solution of (2.2) in *C* corresponding to /? = *fa,* then Lemma 2.2 yields the inequality *Ui* ≤ *m(U\)* at *fa-* Namely *U* is a nontrivial subsolution at /? = *fa.* By Lemma 2.6 we conclude that *faeA.*

Define /3'$_c$ = inf{/? \ *fi* G A}. Then # > 0 (Lemma 2.3) and is the desired critical number described in the first part of the theorem.

The proof for uniqueness of a positive solution is similar to that for the continuous case in [Y] and is skipped here.

To prove the last part of the theorem, we first assume the zero set of *h(k)* in fi is not empty. Let *e* > 0 be sufficiently small so that

$$e < \inf_{\text{kean}} h(k).$$

Let {ft; 11 ≤ *j* ≤ *n]* be a partition of fi with fii = {k G *SI* \ *h(k)* < *e}* and *U* = *{UJ}* a nontrivial solution of (2.2) in *C.* If there is $j_0 \geq 2$ so that *u^* > 0, then (2.2) and the assumption on *K* give us the inequality

$$\begin{aligned} u_j &\geq \min_{\mathbf{k}\in\overline{\Omega}_j,\mathbf{k}'\in\overline{\Omega}_{j_0}} K(\mathbf{k},\mathbf{k}')F_\beta(\mathbf{k}',u_{j_0})u_{j_0}|\Omega_{j_0}| \\ &\geq \min H(k, 10_{\text{fc}} \min h(\mathbf{k}')F_\beta(\mathbf{k}',u_{j_0})u_{j_0}|\Omega_{j_0}| \\ &> 0, \qquad j = 1,2,\cdots,n. \end{aligned}$$

If *Uj* = 0 for all *j* ≥ 2, then using (2.2) again, we have

$$uj = \text{jnin}\ H(k,k')h(k')F_0(k',u\hat{}u\hat{}l = 0, \qquad j = 1,2,.\bullet.,n,$$

which contradicts the nontriviality of *U.* Thus we have shown that *U* is a positive solution.

If the zero set of ^(k) is empty, the function *K* is positive. Then a nontrivial solution in *C* is obviously positive.

Finally, suppose that (2.2) has a nontrivial solution in C at the critical value $\beta = \beta_c'$. Then $U > 0$ as we just observed. Let $\alpha \in (0,1)$ be a fixed number. Since $F_\beta(\mathbf{k}', u)$ is decreasing in $u > 0$, we easily obtain $m(\alpha U) > \alpha U$. This inequality can still be observed when β is slightly below β_c'. In other words, αU is a positive subsolution of (2.2). Hence $\beta \in \Lambda$ (Lemma 2.6), which contradicts the definition of β_c'.

The proof of Theorem 2.1 is complete.

2.2. The max-max scheme

Our next goal is to find upper estimates of a solution and of the critical temperature of (1.1) over Ω. We now introduce the following max-max type discretized approximation.

$$\begin{aligned} U &= \{u_j\} \in \mathbf{R}^n, \\ u_j &= (M(U))_j \\ &\equiv \max_{\mathbf{k}\in\overline{\Omega}_j} \sum_{k=1}^{n} \max_{\mathbf{k}'\in\overline{\Omega}_k} K(\mathbf{k},\mathbf{k}')F_\beta(\mathbf{k}', u_k)u_k|\Omega_k|, \end{aligned} \tag{2.4}$$

Similar to Theorem 2.1, we have

Theorem 2.7. *For any partition $\{\Omega_j \,|\, 1 \le j \le n\}$, there is a number $\beta_c'' > 0$ so that (2.4) for $\beta > \beta_c''$ has a nontrivial solution in C, while for $\beta < \beta_c''$, the only solution of (2.4) in C is the trivial one, $U = 0$. A positive solution is unique. Moreover, partitions of Ω can always be so chosen that a nontrivial solutions of (2.4) in C must be positive, and hence unique, at given $\beta > \beta_c''$. At the critical value $\beta = \beta_c''$, the only solution in C is the zero solution.*

Proof. It is easily seen that Lemmas 2.2–2.3 and 2.5–2.6 are still valid for (2.4) and the operator M. We observe that Lemma 2.4 holds for any partition of Ω. In fact, we have

$$\sum_{k=1}^{n} \max_{\mathbf{k}'\in\overline{\Omega}_k} K(\mathbf{k},\mathbf{k}')F_\beta(\mathbf{k}',\varepsilon)|\Omega_k| \ \ge \int_\Omega K(\mathbf{k},\mathbf{k}')F_\beta(\mathbf{k}',\varepsilon)\,d\mathbf{k}'$$

$$\to \infty \quad \text{as } \varepsilon \to 0 \text{ uniformly in } \mathbf{k} \in \Omega.$$

Thus, parallel to Lemma 2.4, the existence of a critical number β_c'' is ensured for any given partition.

The rest of the proof can be carried out as that for Theorem 2.1. □

2.3. Useful comparisons

Our goal in introducing the schemes (2.2) and (2.4) is to approximate (2.1) defined on a bounded region Ω:

$$\begin{aligned}\Delta(\mathbf{k}) &= (\mathcal{M}_\beta(\Delta))(\mathbf{k}) \\ &= \int_\Omega K(\mathbf{k},\mathbf{k}')F_\beta(\mathbf{k}',\Delta(\mathbf{k}'))\Delta(\mathbf{k}')\,d\mathbf{k}'.\end{aligned} \tag{2.5}$$

Here we have used a subscript to denote the dependence of the BCS operator $\mathcal{M}$ on β. We will use similar notations to indicate the dependence of the operators m and M on β.

It is important to obtain estimates for the critical number β_c of (2.5) so that, for $\beta > \beta_c$, (2.5) has a non-negative solution which is also nontrivial, while for $\beta < \beta_c$, there is only the zero solution.

Viewed as an operator from $C(\overline{\Omega})$ to itself, $\mathcal{M}_\beta$ is clearly Fréchet differentiable and β_c is such that the operator $I - \mathcal{M}_{\beta_c}$ fails to be invertible in a neighborhood of $\Delta = 0$. This fact is equivalent to $\mathrm{Ker}(I - D\mathcal{M}_{\beta_c}(0)) \neq \{0\}$ in view of the Fredholm alternatives and the compactness of $D\mathcal{M}_{\beta_c}(0)$. Namely, β_c is such that the linear integral equation

$$\begin{aligned}u(\mathbf{k}) &= \int_\Omega K(\mathbf{k},\mathbf{k}')F_{\beta_c}(\mathbf{k}',0)u(\mathbf{k}')\,d\mathbf{k}' \\ &= \int_\Omega K(\mathbf{k},\mathbf{k}')\frac{\tanh(\frac{1}{2}\beta_c|\mathbf{k}'^2-\mu|)}{|\mathbf{k}'^2-\mu|}u(\mathbf{k}')\,d\mathbf{k}'\end{aligned}$$

has a nontrivial solution in $C(\overline{\Omega})$, which is an eigenvalue problem. The schemes (2.2) and (2.4) provide upper and lower estimates for such β_c.

Theorem 2.8. *Let $\{\Omega_j \,|\, 1 \leq j \leq n\}$ be a partition of Ω and β_c' and β_c'' are the corresponding critical numbers for (2.2) and (2.4) produced in Theorems 2.1 and 2.7, respectively. Then*

$$\beta_c' \geq \beta_c \geq \beta_c''. \tag{2.6}$$

Besides, if $U = \{u_j\}$, $V = \{v_j\}$, and $\Delta = \Delta(\mathbf{k})$ are maximal solutions of (2.2), (2.4), and (2.5), respectively, then

$$u_j \leq \Delta(\mathbf{k}) \leq v_j \quad \textit{for all } \mathbf{k} \in \overline{\Omega}_j. \tag{2.7}$$

Proof. Of course, $\mathcal{M}_\beta$ can be viewed as an operator defined on $L^\infty(\Omega)$ as well.

For $\beta > \beta_c'$, let $U = \{u_j\}$ be a nontrivial solution of (2.2) in $\mathcal{C}$ and set

$$u(\mathbf{k}) = u_j, \qquad \mathbf{k} \in \Omega_j, \quad j = 1, 2, \cdots, n. \tag{2.8}$$

Then $u \in L^\infty(\Omega)$ and

$$(\mathcal{M}_\beta(u))(\mathbf{k}) \geq (m_\beta(U))_j = u(\mathbf{k}), \qquad \mathbf{k} \in \Omega_j, \quad j = 1, 2, \cdots, n.$$

Thus u is a nontrivial subsolution of (2.5). Consequently, $\beta > \beta_c$, i.e., (2.5) has a nontrivial solution $\Delta(\mathbf{k})$ (say), which can be obtained by iterating from u. Clearly $\beta_c' \geq \beta_c$ and $u \leq \Delta$.

Next, take $\beta > \beta_c$ and assume that Δ is a nontrivial solution of (2.5). Define $\underline{U} = \{\underline{u}_j\} \in \mathcal{C}$ by setting $\underline{u}_j = \max_{\mathbf{k} \in \overline{\Omega}_j} \Delta(\mathbf{k})$. Then

$$\underline{u}_j = \max_{\mathbf{k} \in \overline{\Omega}_j} (\mathcal{M}_\beta(\Delta))(\mathbf{k}) \leq (M_\beta(\underline{U}))_j, \qquad j = 1, 2, \cdots, n$$

due to the definition of M_β (see (2.4)). Hence $\underline{U}$ is a nontrivial subsolution of (2.4). In other words, $\beta > \beta_c''$ and (2.4) has a nontrivial solution, $V = \{v_j\}$, satisfying $\underline{u}_j \leq v_j$. Hence $\beta_c \geq \beta_c''$ and $\Delta(\mathbf{k}) \leq v_j$, $\mathbf{k} \in \Omega_j$, $j = 1, 2, \cdots, n$. □

Let $\mathcal{P} = \{\Omega_j \,|\, 1 \leq j \leq n\}$ and $\mathcal{P}' = \{\Omega_j' \,|\, 1 \leq j \leq n'\}$ be two partitions of Ω. We say that $\mathcal{P}'$ is a refinement of $\mathcal{P}$, written $\mathcal{P} \leq \mathcal{P}'$, if for any $\Omega_j \in \mathcal{P}$ ($j = 1, 2, \cdots, n$), we can find a subcollection of $\mathcal{P}'$ to form a partition of Ω_j.

The dependence of β_c' and β_c'' on the partition $\mathcal{P}$ will be denoted by $\beta_c'(\mathcal{P})$ and $\beta_c''(\mathcal{P})$, respectively. It is readily checked that the definitions of m_β and M_β lead to the inequalities

$$\begin{aligned} \beta_c'(\mathcal{P}) \geq \beta_c'(\mathcal{P}') \geq \beta_c, \\ \beta_c''(\mathcal{P}) \leq \beta_c''(\mathcal{P}') \leq \beta_c, \end{aligned} \qquad \mathcal{P} \leq \mathcal{P}', \tag{2.9}$$

and

$$U_{\mathcal{P}} \leq U_{\mathcal{P}'} \leq \Delta \leq V_{\mathcal{P}'} \leq V_{\mathcal{P}}, \qquad \mathcal{P} \leq \mathcal{P}', \tag{2.10}$$

where Δ is the maximal solution of (2.5) at $\beta > 0$ and $U_{\mathcal{P}}$ ($V_{\mathcal{P}}$) is the maximal solution of (2.2) ((2.4)) corresponding to the partition $\mathcal{P}$ and (2.10) is understood in the space $L^\infty(\Omega)$ with $U_{\mathcal{P}}$ and so on being viewed as measurable functions defined in Ω (see (2.8)).

Recall that β is the inverse of the absolute temperature T. Thus the min-min and the max-max schemes produce two critical temperatures $\tau_c' = 1/\beta_c'$ and $\tau_c'' = 1/\beta_c''$, respectively, so that $\tau_c' \leq T_c \leq \tau_c''$, where $T_c = 1/\beta_c$ is the critical temperature of (2.5). Using the maximal solutions of (2.2) and (2.4), we obtain two functions Δ' and

Δ'' in the space $L^\infty(\Omega)$ according to (2.8). We have seen that $\Delta' \le \Delta \le \Delta''$ where Δ is the maximal solution of (2.5). In the case of positive solutions, these solutions are unique. Thus we conclude that the min-min scheme gives us approximations of the critical temperature and the gap solution of (2.5) from below, while the max-max, from above. The comparison inequalities (2.9) and (2.10) say that finer discretizations always lead to better approximations.

3 Remark on the Full Space Equation

In the last section, we have discussed the approximations of the critical temperature and the nontrivial solutions of the BCS equation (1.1) on a bounded region Ω – the equation (2.5). It seems desirable to expect that, as $\Omega \to \mathbf{R}^3$, the critical temperature on Ω, say $T_c^{(\Omega)}$, will tend to the critical temperature T_c of the full space equation (1.1) on $\mathbf{R}^3$. Moreover, below T_c, a nontrivial solution on $\mathbf{R}^3$ may be obtained from taking the limit $\Omega \to \mathbf{R}^3$ from solutions over Ω. At this moment, we are unable to derive such a general result. However, here, we can establish $T_c^{(\Omega)} \to T_c$ and so on under some sufficiency conditions.

Define

$$\phi_r(\mathbf{k}) = \int_{|\mathbf{k}'|<r} \frac{K(\mathbf{k},\mathbf{k}')}{\mathbf{k}'^2+1}\, d\mathbf{k}', \qquad \phi(\mathbf{k}) = \phi_\infty(\mathbf{k}), \quad \mathbf{k} \in \mathbf{R}^3.$$

Then (1.5) says $\phi_r(\mathbf{k}) \to \phi(\mathbf{k})$ (as $r \to \infty$) uniformly in $\mathbf{R}^3$.

We assume the existence of $r > 0$ and $\alpha > 0$ so that

$$\phi_r(\mathbf{k}) \ge \alpha\phi(\mathbf{k}) \qquad \text{for all } \mathbf{k} \in \mathbf{R}^3. \tag{3.1}$$

Since $\phi_r(k) \le \phi(\mathbf{k})$, we have $\alpha \le 1$. The condition (3.1) was first introduced in [Du] in order to prove the uniqueness of a positive solution of (1.1) over $\mathbf{R}^3$. In this section we show that (3.1) actually provides a connection between full space solutions and solutions over bounded regions of (1.1), therefore, the uniqueness of a positive solution on $\mathbf{R}^3$ is a natural thing to expect. For greater generality, we relax the positivity condition on the kernel function slightly:

$$K(\mathbf{k},\mathbf{k}') = H(\mathbf{k},\mathbf{k}')h(\mathbf{k}'), \quad H(\mathbf{k},\mathbf{k}') > 0, \quad h(\mathbf{k}') \ge 0, \quad \mathbf{k},\mathbf{k}' \in \mathbf{R}^3, \tag{3.2}$$

where H, h are continuous.

Theorem 3.1. *Let $T_c^{(\Omega)} = 1/\beta_c^{(\Omega)}$ and $T_c = 1/\beta_c$ be the critical temperatures of (1.1) on a bounded domain $\Omega \subset \mathbf{R}^3$ and on the full $\mathbf{R}^3$, respectively. Assume (1.5), (3.1), and (3.2). Then*

$$\lim_{\Omega \to \mathbf{R}^3} T_c^{(\Omega)} = T_c. \tag{3.3}$$

More precisely, any nontrivial solution of (1.1) on $\mathbf{R}^3$ must be positive everywhere and can be approximated by taking large domain limit from solutions obtained over bounded domains.

Proof. Let Δ be a nontrivial solution of (1.1) on $\mathbf{R}^3$. Then $\Delta(\mathbf{k}) > 0$ ($\mathbf{k} \in \mathbf{R}^3$). In fact, if there is some $\mathbf{k}_0 \in \mathbf{R}^3$ so that $\Delta(\mathbf{k}_0) = 0$, then (1.1) says $(\mathcal{M}(\Delta))(\mathbf{k}_0) = 0$. However, by (3.2), $h(\mathbf{k}')\Delta(\mathbf{k}') \equiv 0$ ($\mathbf{k}' \in \mathbf{R}^3$), which implies through (1.1) that $\Delta = 0$, a contradiction.

For $r > 0$, define $\Omega_r = \{\mathbf{k} \in \mathbf{R}^3 \mid |\mathbf{k}| < r\}$. Since $F_\beta(\mathbf{k}', u)$ is decreasing in $u \in \mathbf{R}_+$, we have $F_\beta(\mathbf{k}', \alpha\Delta(\mathbf{k}')) > F_\beta(\mathbf{k}', \Delta(\mathbf{k}'))$ for any $\alpha \in (0,1)$. Using this fact in (1.1), we obtain $\mathcal{M}(\alpha\Delta) > \alpha\Delta$. We hope to generalize the above inequality into the form

$$\mathcal{M}^{(\Omega_r)}(\alpha\Delta_r) > \alpha\Delta_r, \qquad \mathbf{k} \in \Omega_r, \tag{3.4}$$

where $r > 0$ is sufficiently large,

$$\begin{aligned} \mathcal{M}^{(\Omega_r)}(u)(\mathbf{k}) &= \int_{\Omega_r} K(\mathbf{k}, \mathbf{k}')\varphi_\beta(\mathbf{k}', u(\mathbf{k}'))\, d\mathbf{k}', \\ \Delta_r(\mathbf{k}) &= \int_{\Omega_r} K(\mathbf{k}, \mathbf{k}')\varphi_\beta(\mathbf{k}', \Delta(\mathbf{k}'))\, d\mathbf{k}'. \end{aligned}$$

Of course, $\Delta_r = \mathcal{M}^{(\Omega_r)}(\Delta)$.

Put $R(\mathbf{k}, r) = \alpha\Delta_r(\mathbf{k}) - \mathcal{M}^{(\Omega_r)}(\alpha\Delta_r)(\mathbf{k})$. To prove (3.4), we need to show the existence of an $r_0 > 0$ so that $R(\mathbf{k}, r) < 0$ for $\mathbf{k} \in \Omega_r$ whenever $r \geq r_0$. We decompose $R(\mathbf{k}, r)$ as follows.

$$R(\mathbf{k}, r) = R_1(\mathbf{k}) + R_2(\mathbf{k}, r) + R_3(\mathbf{k}, r), \tag{3.5}$$

where

$$\begin{aligned} R_1(\mathbf{k}) &= \alpha\Delta(\mathbf{k}) - \mathcal{M}(\alpha\Delta)(\mathbf{k}), \\ R_2(\mathbf{k}, r) &= \mathcal{M}(\alpha\Delta)(\mathbf{k}) - \mathcal{M}(\alpha\Delta_r)(\mathbf{k}), \\ R_3(\mathbf{k}, r) &= [\mathcal{M}(\alpha\Delta_r)(\mathbf{k}) - \mathcal{M}^{(\Omega_r)}(\alpha\Delta_r)(\mathbf{k})] - \alpha[\mathcal{M}(\Delta)(\mathbf{k}) - \mathcal{M}^{(\Omega_r)}(\Delta)(\mathbf{k})]. \end{aligned}$$

For $R_1(\mathbf{k})$, we have

$$\begin{aligned} R_1(\mathbf{k}) &= \alpha \int_{\mathbf{R}^3} K(\mathbf{k},\mathbf{k}')[F_\beta(\mathbf{k}',\Delta(\mathbf{k}')) - F_\beta(\mathbf{k}',\alpha\Delta(\mathbf{k}'))]\Delta(\mathbf{k}')\,d\mathbf{k}' \\ &< \alpha \int_{|\mathbf{k}'|<r} K(\mathbf{k},\mathbf{k}')[F_\beta(\mathbf{k}',\Delta(\mathbf{k}')) - F_\beta(\mathbf{k}',\alpha\Delta(\mathbf{k}'))]\Delta(\mathbf{k}')\,d\mathbf{k}' \\ &= -\alpha \int_{|\mathbf{k}'|<r} K(\mathbf{k},\mathbf{k}')\varphi_\beta(\mathbf{k}',\Delta(\mathbf{k}'))\left[\frac{F_\beta(\mathbf{k}',\alpha\Delta(\mathbf{k}'))}{F_\beta(\mathbf{k}',\Delta(\mathbf{k}'))} - 1\right] d\mathbf{k}' \\ &\le -\alpha\delta_1(r)\Delta_r(\mathbf{k}), \end{aligned} \tag{3.6}$$

where

$$\delta_1(r) = \inf_{|\mathbf{k}'|<r} \left[\frac{F_\beta(\mathbf{k}',\alpha\Delta(\mathbf{k}'))}{F_\beta(\mathbf{k}',\Delta(\mathbf{k}'))} - 1\right] > 0.$$

For $R_2(\mathbf{k},r)$, we have

$$\begin{aligned} R_2(\mathbf{k},r) &= \alpha \int_{\mathbf{R}^3} K(\mathbf{k},\mathbf{k}')[F_\beta(\mathbf{k}',\alpha\Delta(\mathbf{k}'))\Delta(\mathbf{k}') - F_\beta(\mathbf{k}',\alpha\Delta_r(\mathbf{k}'))\Delta_r(\mathbf{k}')]\,d\mathbf{k}' \\ &\le \alpha \int_{\mathbf{R}^3} K(\mathbf{k},\mathbf{k}')F_\beta(\mathbf{k}',\alpha\Delta(\mathbf{k}'))(\Delta(\mathbf{k}') - \Delta_r(\mathbf{k}'))\,d\mathbf{k}' \\ &\le C_2\delta_2(r)\phi(\mathbf{k}), \end{aligned} \tag{3.7}$$

where $C_2 > 0$ is a constant independent of $r > 0$ and

$$\delta_2(r) = \sup_{\mathbf{k}\in\mathbf{R}^3} (\Delta(\mathbf{k}) - \Delta_r(\mathbf{k})) \to 0 \quad \text{as } r \to \infty$$

due to (1.5). For $R_3(\mathbf{k},r)$, we have

$$\begin{aligned} R_3(\mathbf{k},r) &= \int_{|\mathbf{k}'|\ge r} K(\mathbf{k},\mathbf{k}')[\varphi_\beta(\mathbf{k}',\alpha\Delta_r(\mathbf{k}')) - \alpha\varphi_\beta(\mathbf{k}',\Delta(\mathbf{k}'))]\,d\mathbf{k}' \\ &\le \int_{|\mathbf{k}'|\ge r} K(\mathbf{k},\mathbf{k}')[\varphi_\beta(\mathbf{k}',\alpha\Delta(\mathbf{k}')) - \alpha\varphi_\beta(\mathbf{k}',\Delta(\mathbf{k}'))]\,d\mathbf{k}' \\ &= \alpha \int_{|\mathbf{k}'|\ge r} K(\mathbf{k},\mathbf{k}')\varphi_\beta(\mathbf{k}',\Delta(\mathbf{k}'))\left[\frac{F_\beta(\mathbf{k}',\alpha\Delta(\mathbf{k}'))}{F_\beta(\mathbf{k}',\Delta(\mathbf{k}'))} - 1\right] d\mathbf{k}' \\ &\le \alpha\delta_3(r)(\Delta(\mathbf{k}) - \Delta_r(\mathbf{k})) \le \alpha\delta_3(r)\Delta(\mathbf{k}), \end{aligned} \tag{3.8}$$

where

$$\delta_3(r) = \sup_{|\mathbf{k}'|\ge r} \left[\frac{F_\beta(\mathbf{k}',\alpha\Delta(\mathbf{k}'))}{F_\beta(\mathbf{k}',\Delta(\mathbf{k}'))} - 1\right] \to 0 \quad \text{as } r \to \infty.$$

In view of (1.5), we easily see that there is a constant $C_3 > 0$ so that $\Delta(\mathbf{k}) \leq C_3\phi(\mathbf{k})$ ($\mathbf{k} \in \mathbf{R}^3$). Thus (3.8) becomes

$$R_3(\mathbf{k}, r) \leq \alpha C_3 \delta_3(r)\phi(\mathbf{k}), \qquad \mathbf{k} \in \mathbf{R}^3. \tag{3.9}$$

On the other hand, setting

$$\delta_0(r) = \inf_{|\mathbf{k}|<r} \Delta(\mathbf{k}) > 0,$$

we obtain

$$\begin{aligned} \Delta_r(\mathbf{k}) &\geq \int_{|\mathbf{k}'|<r} K(\mathbf{k}, \mathbf{k}')\varphi_\beta(\mathbf{k}', \delta_0(r))\, d\mathbf{k}' \\ &\geq C_1(r)\phi_r(\mathbf{k}) \geq \gamma C_1(r)\phi(\mathbf{k}) \end{aligned} \tag{3.10}$$

by (3.1), where

$$C_1(r) = \inf_{|\mathbf{k}'|<r} \{(\mathbf{k}'^2 + 1)\varphi_\beta(\mathbf{k}', \delta_0(r))\} > 0.$$

The inequalities (3.6) and (3.10) imply

$$R_1(\mathbf{k}) \leq -\alpha\gamma\delta_1(r')C_1(r')\phi(\mathbf{k}), \tag{3.11}$$

where $r' > 0$ is sufficiently large and is fixed. Inserting (3.11), (3.7), and (3.9) into (3.5), we get

$$R(\mathbf{k}, r) \leq -(\alpha\gamma\delta_1(r')C_1(r') - C_2\delta_2(r) - \alpha C_3\delta_3(r))\phi(\mathbf{k}).$$

Therefore $R(\mathbf{k}, r) < 0$ when $r > 0$ is large, since $\delta_2(r), \delta_3(r) \to 0$ as $r \to \infty$. Thus our early assertion is proved. Namely, (3.4) holds.

The inequality (3.4) says that $\alpha\Delta_r$ is a positive subsolution of (2.5) on $\Omega = \Omega_r$, or equivalently, (2.5) has a positive solution, $\Delta^{(\Omega_r)}$ (say). Such a solution is of course unique [Y].

Let $\{\Omega_j \,|\, j = 1, 2, \cdots\}$ be a monotone chain of bounded domains in $\mathbf{R}^3$ with $\cup_{j=1}^{\infty} \Omega_j = \mathbf{R}^3$. Then

$$T_c^{(\Omega_1)} \leq T_c^{(\Omega_2)} \leq \cdots \leq T_c^{(\Omega_j)} \leq \cdots \leq T_c$$

(see [Y]). Set $T_\infty = \lim_{j\to\infty} T_c^{(\Omega_j)}$. We claim that $T_\infty = T_c$. Indeed, if $T_\infty < T_c$, then (1.1) has a positive solution in $\mathbf{R}^3$ at any $T = 1/\beta : T_\infty < T < T_c$. By the above discussion, we can find an $r > 0$ so that (2.5) has a positive solution at $\beta = 1/T$ for $\Omega = \Omega_r$. Namely, $T_\infty < T < T_c^{(\Omega_r)}$. However, there is a $j \geq 1$ so that $\Omega_r \subset \Omega_j$ and $T_c^{(\Omega_r)} \leq T_c^{(\Omega_j)}$. Therefore $T^{(\Omega_r)} \leq T_\infty$, a contradiction. So the claim, hence (3.3), is proved. This argument also shows that, whenever (1.1) has a nontrivial solution at $T = 1/\beta$, then $T < T_c^{(\Omega_j)}$ for large j.

Thus, at T, let $\Delta^{(\Omega_j)}$ be a nontrivial solution of (2.5) on $\Omega = \Omega_j$ (if it exists), $j = 1, 2, \cdots$. We assume the convention $\Delta^{(\Omega_j)}(\mathbf{k}) = 0$ for $\mathbf{k} \in \mathbf{R}^3 - \Omega_j$. The sequence $\{\Delta^{(\Omega_j)}\}$ is nontrivial and monotone increasing

$$\Delta^{(\Omega_1)} \leq \Delta^{(\Omega_2)} \leq \cdots \leq \Delta^{(\Omega_j)} \leq \cdots. \tag{3.12}$$

We now derive the following pointwise convergence property

$$\lim_{j \to \infty} \Delta^{(\Omega_j)}(k) = \Delta(\mathbf{k}), \qquad \mathbf{k} \in \mathbf{R}^3. \tag{3.13}$$

In fact, $\Delta^{(\Omega_j)}$ is a sequence of subsolutions of (1.1) and, thus, is bounded [Y]. Consequently the pointwise limit, say $\Delta_\infty(\mathbf{k})$, on the left-hand side of (3.13), exists in view of (3.12). It is straightforward to examine that Δ_∞ is a solution of (1.1) in $\mathbf{R}^3$.

We have shown that for any $\alpha \in (0,1)$, $\alpha\Delta_r$ is a positive subsolution of (2.5) on $\Omega = \Omega_r$ when $r > 0$ is sufficiently large. Thus the existence of a positive solution, $\Delta^{(\Omega_r)}$, of (2.5) for $\Omega = \Omega_r$ is ensured. Let $j \geq 1$ be such that $\Omega_r \subset \Omega_j$. Then $\Delta^{(\Omega_r)} \leq \Delta^{(\Omega_j)}$. In particular, $\alpha\Delta_r(\mathbf{k}) \leq \Delta_\infty(\mathbf{k})$. However, α can chosen arbitrarily close to 1 and r arbitrarily large, thus $\Delta(\mathbf{k}) \leq \Delta_\infty(\mathbf{k})$, $\mathbf{k} \in \mathbf{R}^3$. On the other hand, since $\alpha\Delta_r < \Delta$ and $\alpha\Delta_r$ is a positive subsolution and Δ a supersolution of (2.5) on $\Omega = \Omega_r$, we have $\Delta^{(\Omega_r)} \leq \Delta$ in Ω_r. Given $j \geq 1$, let $r > 0$ be large so that $\Omega_j \subset \Omega_r$. Then $\Delta^{(\Omega_j)} \leq \Delta^{(\Omega_r)}$. Hence $\Delta^{(\Omega_j)} \leq \Delta$. This proves that $\Delta_\infty \leq \Delta(\mathbf{k})$, $\mathbf{k} \in \mathbf{R}^3$. Thus $\Delta = \Delta_\infty$.

The proof also shows the uniqueness of a positive solution in the full space $\mathbf{R}^3$. □

4 Numerical Examples

For convenience, we shall adapt slightly different notation in this section to present some discussion of the discretized equations. Using the results in Section 2, we have implemented the following monotone iterations to approximate the solutions of the BCS equation and to estimate the critical temperatures:

1 Min-min iteration

$$\begin{aligned} U_{min}^{l+1} &= \{u_j\} \in \mathbf{R}^n, U_{min}^l = \{v_j\} \in \mathbf{R}^n, \text{ where} \\ u_j &\equiv \min_{\mathbf{k} \in \bar{\Omega}_j} \sum_{k=1}^{n} \min_{\mathbf{k}' \in \bar{\Omega}_k} K(\mathbf{k}, \mathbf{k}') F_\beta(\mathbf{k}', v_k) v_k |\Omega_k|, \end{aligned} \tag{4.1}$$

2 Max-max iteration

$$U^{l+1}_{max} = M \in \mathbf{R}^n, U^l_{max} = \{v_j\} \in \mathbf{R}^n, \quad \text{where}$$

$$u_j \equiv \max_{\mathbf{k}\in\overline{\Omega}_j} \sum_{k=1}^{n} \max_{\mathbf{k}'\in\overline{\Omega}_k} K(\mathbf{k},\mathbf{k}')F_\beta(\mathbf{k}',v_k)v_k|\Omega_k|, \tag{4.2}$$

The convergence of the above iterations has been shown in Section 2. To initiate the iterations, we start with a constant state with value 6_0 which is chosen by

$$\max_{1\le j\le n} \max_{\mathbf{k}\in\overline{\Omega}_j} \sum_{k=1}^{n} \max_{\mathbf{k}'\in \mathrm{H}_k} K(k,k^f)FQ(k^f,6_0)\backslash n_k\backslash < 1 \ . \tag{4.3}$$

It is obvious that this constant state is a supersolution of the min-min and the max-max iteration for any positive values of /?.

Thus, in principle, we can use the constant state for all values of *f3* and iterate until the iteration converges. In actual computation, we proceed with the iteration for various values of /? that are taken to be in decreasing order so that the solution corresponding to the previous, larger value of /? becomes a supersolution for the smaller values of /?. In other words, a continuation in the parameter /? is used which reduces the total number of the iterations needed, comparing with starting at constant state for any /?.

Meanwhile, calculations using different partitions of the region are used to obtain accurate estimates of the critical temperatures.

For simplicity, we shall restrict our attention to the spherically symmetric case where the kernel function depends only on the radial variables $x = |\mathrm{k}|$ and $y = |\mathrm{k}'|$. After an obvious normalization, the BCS equation (1.1) is reduced to

$$\Delta(x) = \int_0^{r_0} K(x,y)\frac{\tanh(\frac{1}{2}\beta((y^2-\mu)^2+\Delta^2(y))^{1/2})}{((y^2-\mu)^2+\Delta(y))^{1/2}}\Delta(y)\,dy,$$

where r_0 > *yfji* > 0 is a suitable truncation barrier for the energy level in the model. To be specific in our numerical examples, we fix a choice of the symmetric kernel function *K(x^y)* so that

$$K(x,y) = \frac{2V\alpha}{\pi}\frac{y^2}{[\alpha^2 + (x + J/)^2][a^* + (x - yp]} * \tag{4.4}$$

Such a model arises in the physical situation that the interaction potential is of a Yukawa type, $Ve^{\sim Qr}$. See [BF] and references therein. It is easily checked that the equation here satisfies all the good conditions given in Section 2 when we specialize in the one-dimensional setting stated above. Thus both the continuous and discretized

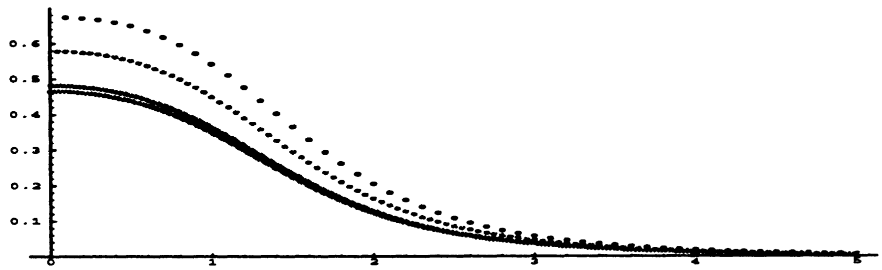

Figure 1: The solution U_{max} at $\beta = 5.0, V = 1.0$ with various partitions (From top down, N = 50, 100, 500 and 2000)

BCS equations ((2.5), (2.2), (2.4)) have unique positive solutions below their critical temperatures (a positive critical temperature for the min-min equation exists if the discretization is fine enough).

In all the reported calculations to follow, we take $\mu = 1$, $\alpha = 1$, and $r_0 = 5$. Those values are only chosen as an illustration and may not correspond to any realistic physical situation. The interval $(0, r_0) = (0, 5)$ is uniformly partitioned into small intervals. We use N to denote the number of grid points.

First, we compare the solutions for a given value of β, $\beta = 5.0$ ($T = 0.2$).

From Figures 1 and 2, one can observe the fact that for given values of β and V, the solution of the max-max iteration for a partition with smaller number of grid points is a supersolution for a partition with larger number of grid points, since the latter is a refinement of the former. Similarly, the solution of the min-min iteration for a partition with smaller number of grid points is a subsolution for a partition with lager number of grid points.

Figure 3 gives a comparison between the solutions of the max-max iteration and the min-min iteration with the same number of grid points used in the partition ($N = 2000$).

Next, in Figures 4 and 5, we compare the solution with various values of β with respect to a given partition $N = 500$. Here, $V = 1.0$.

Next, we plot in figure 6 the approximate values of U_{max} and U_{min} at the point

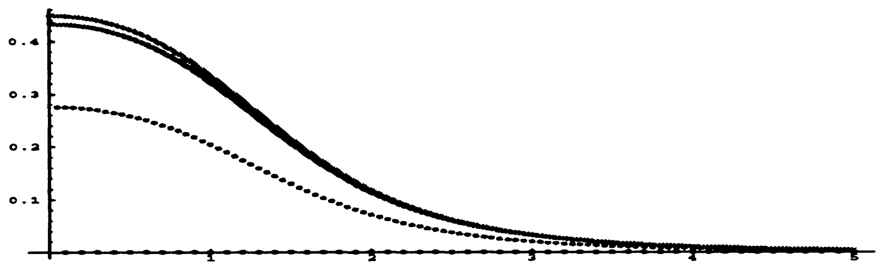

Figure 2: The solution U_{min} at $\beta = 5.0, V = 1.0$ with various partitions (From bottom up, $N = 50$, 100, 500 and 2000)

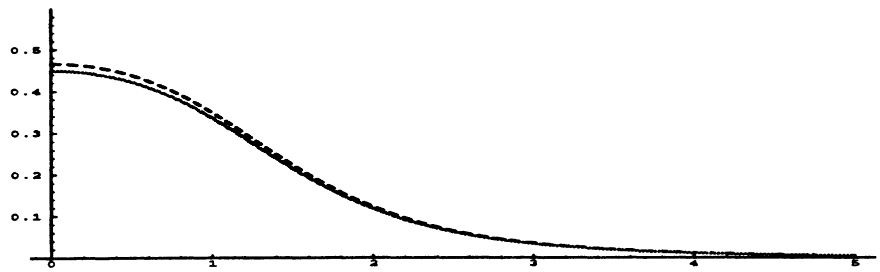

Figure 3: The solutions U_{max} (– – –) and U_{min} (——) at $\beta = 5.0, V = 1.0$ with $N = 2000$

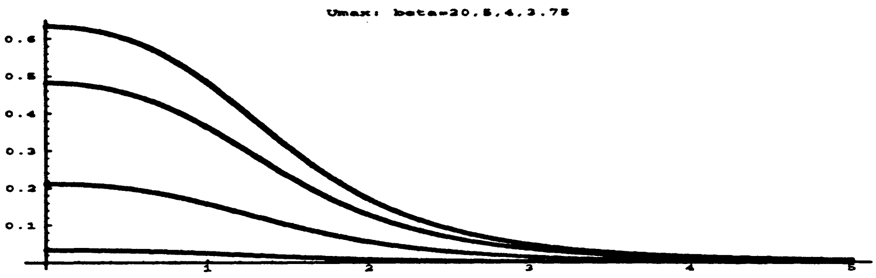

Figure 4: The solution U_{max} with various values of β (From top down, $\beta = 20, 5, 4$ and 3.75)

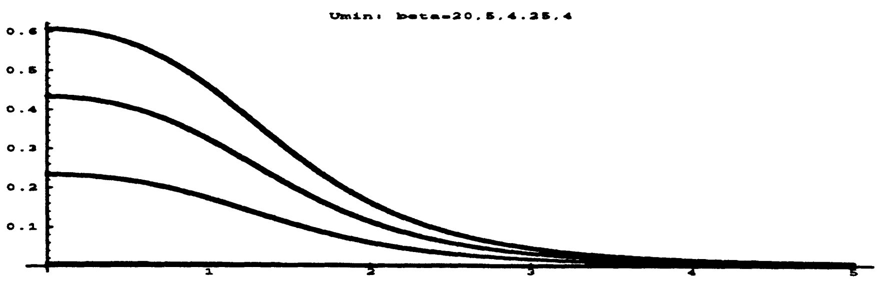

Figure 5: The solution U_{min} with various values of β (From top down, $\beta = 20, 5, 4.25$ and 4)

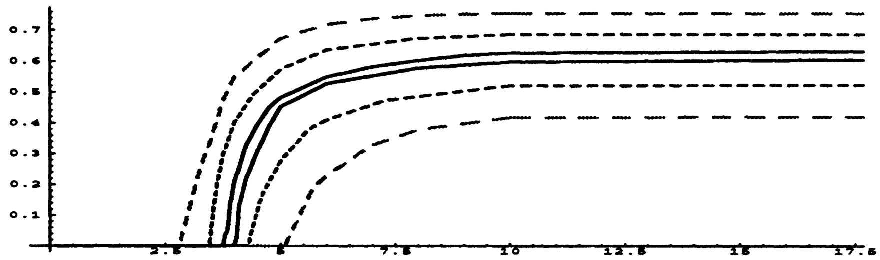

Figure 6: The values of $U_{max}(0)$ and $U_{min}(0)$ vs. values of β. (From left to right, $U_{max}(0)$ for $N = 50, 100, 500$ and $U_{min}(0)$ for $N = 500, 100, 50$)

$x = 0$ against values of β. Notice that at $x = 0$, solutions have their maximum values. Here again, $V = 1.0$ and the figures shows that the approximate critical temperature is around 0.26.

Finally, we also provide a few plots with a different value of V, this change effectively make the critical temperature much larger. Figure 7 gives the plot of the values of solution at $x = 0$ against the values of temperature $T = 1/\beta$. In this case, T_c is approximately 10.7.

Figures 8 and 9 provide data on the number of iterations used in performing the min-min and max-max iterations against various values of β. Note that the darker area (top area) represents additional iterations starting with the solution corresponding to the previous value of β. It is worthwhile to note that as β goes closer and closer to its critical value, the number of iterations becomes larger and larger. It also implies that other algorithms may need to be implemented at or very near the critical temperature to ensure efficient numerical procedures.

References

[BF] P. Billard and G. Fano, An existence proof for the gap equation in the superconductivity theory, *Commun. Math. Phys.* **10**, 274-279, (1968).

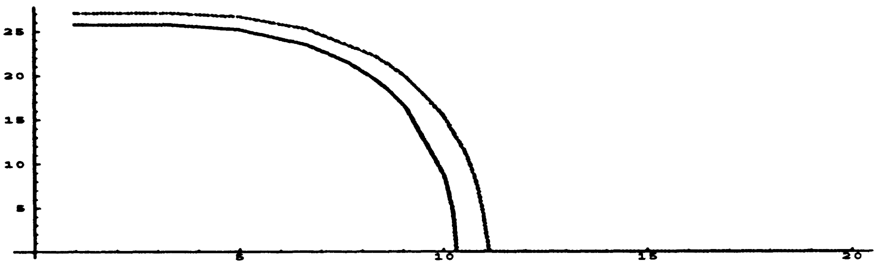

Figure 7: The values of $U_{max}(0)$ (top) and $U_{min}(0)$ (bottom) vs. T ($N = 100$).

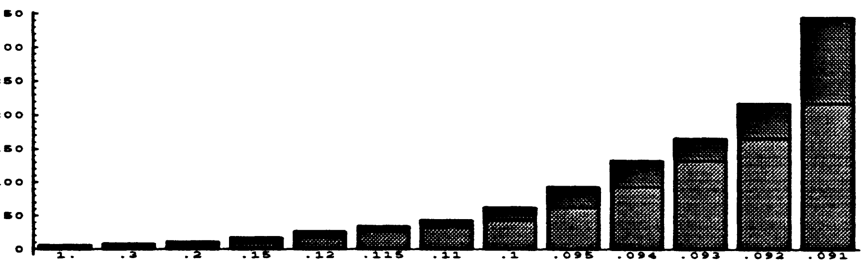

Figure 8: The number of max-max iteration against values of β with $N = 100$

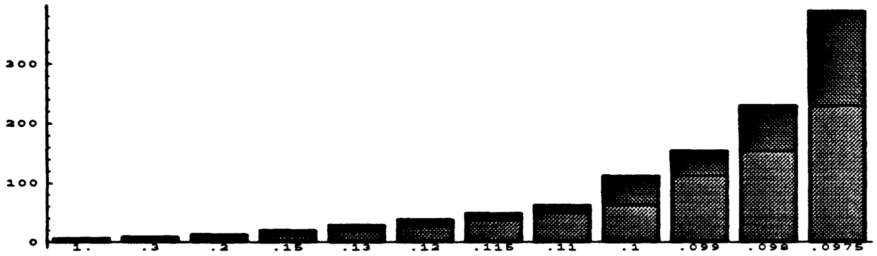

Figure 9: The number of min-min iteration against values of β with $N = 100$

[D] A. S. Davydov, Theoretical investigation of high-temperature superconductivity, *Phys. Rep.* **190**, 191–306 (1990).

[Du] Y. Du, Uniqueness results for the gap equation in the theory of superconductivity, *Preprint*, 1992.

[E] C. P. Enz, Introduction to the physics of high-temperature superconductors, *Helv. Phys. Acta* **61**, 741–759 (1988).

[H] N. M. Hugenholtz, Quantum theory of many-body systems, *Rep. Progr. Phys.* **28**, 201–247 (1965).

[vH] L. van Hemmen, Linear fermion systems, molecular field models, and the KMS condition, *Fortschr. Phys.* **26**, 379–439 (1978).

[K] M. Kitamura, Nonlinear integral equation of the Hammerstein type, *Progr. Theoret. Phys.* **30**, 435–442 (1963).

[WE] M. Weger and R. Englman, A dynamic Jahn–Teller theory for high-T_c superconductivity, *Physica A* **168**, 324–337 (1990).

[WEH] M. Weger, R. Englman, and B. Halperin, Oscillatory solutions of the BCS gap equation, *Solid State Commun.* **71**, 17–72 (1988).

[Y] Y. Yang, On the Bardeen–Cooper–Schrieffer integral equation in the theory of superconductivity, *Lett. Math. Phys.* **22**, 27–37 (1991).