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Investigation of non-magnetic impurity doping effect on the MgB_2 superconductor critical temperature

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Abstract
We have investigated the effect of finite non-magnetic impurity doping concentration on the critical temperature (T_c) of the MgB_2 superconductor by using the coherent potential approximation. We found, by choosing the chemical potential $\mu = -0.47t$ and scattering strength $\delta = 4.5t$, that T_c is reduced with impurity concentration similarly to the measured experimental results.

1. Introduction

The discovery of superconductivity with a transition temperature of 39 K in a binary metallic compound of MgB_2 [1] has attracted great interest from scientists all over the world because of its high transition temperature. In the early stage of superconductive material investigation, several inter-metallic material groups including the AlB_2-type structure were already recognized as candidate materials for 'high-T_c' superconductors, mainly by Matthias and Hulm in the 1950s. 'Matthias's rule' was derived through the investigation of $A1_5$-type superconductors [2] such as Nb_3Sn, V_3Ga, $Nb_3(AlGe)_2$ and Nb_3Ge_3, which are important for practical applications. The superconductors discovered in this stage are called 'BCS superconductors' because their behavior can be well explained within the framework of the BCS (Bardeen–Cooper–Schrieffer) theory. Most studies performed on this compound indicate that MgB_2 consistently behaves as a phonon-mediated superconductor within the framework of the BCS theory, probably in a strong coupling limit [3, 4]. The transition temperature is surprisingly high for a non-cuprate material, and much above the limit expected for a classical superconducting compound. The observation of a boron isotope effect on T_c suggests a phonon-mediated pairing mechanism [3]. In the BCS theory [5], T_c scales with the Debye energy when the effective attractive interaction between electrons is due to phonons.

The effects of impurities in this material are very interesting to study. According to Anderson's theorem (AT) for classic s-wave superconductors [6–8], non-magnetic impurities do not affect superconducting properties in zero magnetic field. However, it was shown later by Markowitz and Kadanoff [9] that T_c is actually reduced in the presence of gap anisotropy and impurity scattering. Also, we have shown [10] that, for low impurity concentrations c and weak on-site energies, AT is valid, while in the strong scattering limit T_c is very small even for low c, and it is completely suppressed by increasing c; hence AT is violated in this regime. An application of a two-band model is due to Golubov and Mazin [11]. Indeed, they predicted a rather drastic decrease in T_c due to interband impurity scattering. They also found that, as the interband scattering increases, the density of states changes from the two-gap structure inherent in the two-band model to the conventional single-gap structure. This reduction in T_c has been confirmed recently by a couple of experiments. Wang *et al* [12] measured the specific heat of polycrystalline MgB_2 after irradiation. They found both the suppression of T_c and a tendency towards a single-gap structure as scattering is increased by irradiation. Lee *et al* [13] clarified the possibility of the complete suppression of superconductivity by replacing B in MgB_2 by C. However, few quantitative calculations have been performed on the impurity effects based on a realistic model for MgB_2 [14]. To study the influence of electron doping on the Mg site in MgB_2, Slusky *et al* [15] investigated the substitution of Al for Mg to synthesize $MgB_{1-x}Al_xB_2$ and found that their samples lose superconductivity when x was near about 0.4. Zhang *et al* [16], Kazakov *et al* [17] and Rogacki *et al* [18] studied the superconductivity of $Mg(B_{1-x}C_x)_2$ and found that the transition temperature of

their samples decreases when they were doped with carbon powder. We investigated the effects of non-magnetic impurity doping on the reduction in the critical temperature, T_c, of MgB_2 superconductor to explain the experimental results of [17, 18]. We calculated T_c in terms of the impurity doping concentration, in agreement with the experimental data in [17, 18]. In section 2, we introduce the model and obtain the equation of motion. In section 3, by using the coherent potential approximation (CPA), we solve the equation of motion and calculate T_c. In the last section, we present the numerical results.

2. Model and formalism

MgB_2 has the AlB_2-type structure. It is composed of two layers of boron and magnesium along the c-axis in the hexagonal lattice with $a = 3.08$ and $c = 3.51$ Å (hexagonal: space group $P6/mmm$). In this structure, the characteristic two-dimensional (2D) honeycomb layers formed by boron atoms are sandwiched by the triangular metal layers, like intercalated graphite. Each Mg atom is at the center of a hexagonal prism of boron atoms at a distance of 2.5 Å. Each boron atom is surrounded by three other boron atoms, forming an equilateral triangle at a distance of $a_0 = \frac{a}{\sqrt{3}} \sim 1.78$ Å, while the Mg–Mg distance in the plane is equal to the lattice constant a. Because lattice constants a and c in the AlB_2-type structure are in the range 3.0–3.2 Å and 3.0–4.0 Å, respectively, MgB_2 has an intermediate lattice constant among this type of structure. The two electrons belonging to the Mg atom transfer to B_2, and the former changes to Mg^{2+} while the latter becomes B^{2-}. The B_2 ions become metallic by obtaining two electrons, and Mg ions become insulating by losing two electrons. It has also been shown experimentally by Takahashi *et al* [19] using photoemission spectroscopy that the B_2 plane is superconducting. Thus we assume that MgB_2 consists of 2D B_2 superconductors with weak Cooper pair interaction arranged in parallel planes normal to the direction of the c-axis.

We start our investigation with the following random extended attractive Hubbard model on a three-dimensional hexagonal lattice,

$$H = -\sum_{ij\sigma\alpha\beta} t_{i\sigma j\sigma}^{\alpha\beta} c_{i\sigma}^{\alpha\dagger} c_{j\sigma}^{\beta} + \sum_{ij\sigma\alpha} U_{ij} \hat{n}_{i\sigma}^{\alpha} \hat{n}_{i-\sigma}^{\alpha} + \sum_{i\sigma\alpha} (\varepsilon_i^{\alpha} - \mu) \hat{n}_{i\sigma}^{\alpha}, \tag{1}$$

where α and β refer to the two non-equivalent sites, A or B, in the graphite-like unit cell (figure 1), ${c^{\alpha}}_{i\sigma}^{\dagger}$ ($c_{i\sigma}^{\alpha}$) is the creation (annihilation) operator of an electron with spin σ on Bravais lattice site i, and $\hat{n}_{i\sigma}^{\alpha} = {c^{\alpha}}_{i\sigma}^{\dagger} c_{i\sigma}^{\alpha}$ is the number operator. $t_{i\sigma j\sigma}^{\alpha\beta}$ are the hopping integrals between sites i and j with spin σ. U_{ij} is the attractive interaction potential between electrons of opposite spins at sites i and j. μ is the chemical potential, and ε_i^{α} is the random on-site energy, which takes value 0 with probability $1 - c$ for host sites (boron host sites) and δ with probability c for impurity sites (related to the carbon impurities).

In the weak interaction regime, for any given configuration of impurity sites the solution of equation (1) is given by the Bogoliubov–de Gennes equation where, for singlet-state superconductors, the order parameter, $\Delta_{ij}^{\sigma\sigma'} = \frac{U_{ij}^{\sigma\sigma'}}{\beta} \sum_n G^{\sigma\sigma'}(i, j; \mathrm{i}\omega_n)$, of Cooper pairs with same spins are zero $\Delta_{ij}^{\uparrow\uparrow} = \Delta_{ij}^{\downarrow\downarrow} = 0$ and $\Delta_{ij}^{\uparrow\downarrow} = \Delta_{ij}^{\downarrow\uparrow} = \Delta_{ij}$,

$$\sum_l \begin{pmatrix} (E + \varepsilon_i + \mu_{i\downarrow})\delta_{il} + t_{il}^{AA} & \Delta_{il} & t_{il}^{AB} & 0 \\ \Delta_{il}^{*} & (E - \varepsilon_i - \mu_{i\uparrow})\delta_{il} - t_{il}^{AA} & 0 & -t_{il}^{AB} \\ t_{il}^{BA} & 0 & (E + \varepsilon_i + \mu_{i\downarrow})\delta_{il} + t_{il}^{BB} & \Delta_{il} \\ 0 & -t_{il}^{BA} & \Delta_{il}^{*} & (E - \varepsilon_i - \mu_{i\uparrow})\delta_{il} - t_{il}^{BB} \end{pmatrix} \times \mathbf{G}(l, j; E) = \mathbf{I}\delta_{ij}, \tag{2}$$

where $\mu_{i\sigma} = \mu - U_i n_{i-\sigma}$ is the on-site renormalized chemical potential due to the usual Hartree decoupling, $\Delta_{il} = \Delta_{il}^0 + \delta\Delta_{il}$ where Δ_{il}^0 is the clean system order parameter and $\delta\Delta_{il}$ is the spatial deviation of the order parameter, and $t_{i\sigma l\sigma}^{\alpha\beta}$ is denoted by $t_{il}^{\alpha\beta}$. The coupling parameters U_{ij} and order parameters Δ_{ij} have non-zero values only for two cases: $U_i^{\parallel}$ and $\Delta_i^{\parallel}$ if the sites i and j coincide in a B_2 plane, and $U_{\langle ij\rangle}^{\perp}$ and $\Delta_{\langle ij\rangle}^{\perp}$ if i and j are nearest neighbors in adjacent B_2 planes. U_{ij} and Δ_{ij} defined as,

$$\Delta_{ij} = \Delta_{ij}^{\parallel} + \Delta_{ij}^{\perp}, \tag{3}$$

$$U_{ij} = U_{ij}^{\parallel} + U_{ij}^{\perp}. \tag{4}$$

For first nearest neighbor inter planes, the local order parameter intra plane and local interaction potential intra plane, equations (3) and (4) can be written as,

$$\Delta_{ij} = \Delta_i^{\parallel}\delta_{ij} + \Delta_{\langle ij\rangle}^{\perp}, \tag{5}$$

$$U_{ij} = U_i^{\parallel}\delta_{ij} + U_{\langle ij\rangle}^{\perp}. \tag{6}$$

We suppose that these local quantities do not change appreciably on length scales $\sim\frac{1}{k}$ so, by writing the Fourier transform of order parameters, we have,

$$\Delta^{\perp}(\mathbf{k}) = \frac{1}{N}\sum_{\langle ij\rangle} \Delta_{\langle ij\rangle}^{\perp} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_{\langle ij\rangle}} = 2\Delta_{\langle ij\rangle}^{\perp}\cos(ck_z), \tag{7}$$

$$\Delta^{\parallel}(\mathbf{k}) = \Delta_i^{\parallel}, \tag{8}$$

so we find the gap function in the form,

$$\Delta(\mathbf{k}) = \Delta_i^{\parallel} + 2\Delta_{\langle ij\rangle}^{\perp}\cos(ck_z). \tag{9}$$

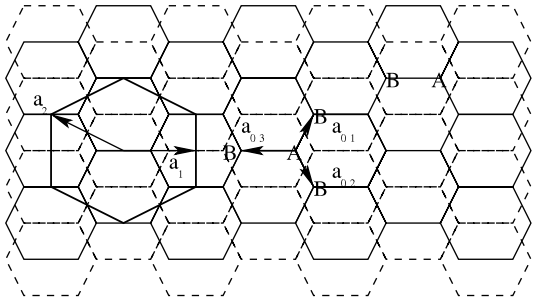

Figure 1. A two-dimensional graphite-like (B_2) sheet. The light dashed lines illustrate the Bravais lattice unit cells; $\mathbf{a}_1$ and $\mathbf{a}_2$ are the primitive vectors. Each cell includes two non-equivalent sites, which are denoted by A and B.

By assuming that the order parameter is real, we obtain,

$$\Delta_i^{\parallel} = -\frac{U_i^{\parallel}}{\pi}\int_{-\infty}^{+\infty} \mathrm{d}Ef(E)\,\mathrm{Im}\,G_{12}^{AA\uparrow\downarrow}(i,i;E), \tag{10}$$

$$\Delta_{\langle ij\rangle}^{\perp} = -\frac{U_{\langle ij\rangle}^{\perp}}{\pi}\int_{-\infty}^{+\infty} \mathrm{d}Ef(E)\,\mathrm{Im}\,G_{12}^{AA\uparrow\downarrow}(i,j;E), \tag{11}$$

and the local band filling, n_i, is

$$n_i = 2\int_{-\infty}^{+\infty} \mathrm{d}Ef(E)\,\mathrm{Im}\,G_{11}^{AA\uparrow\uparrow}(i,i;E), \tag{12}$$

where $f(E) = \frac{1}{\mathrm{e}^{\frac{E}{k_BT}}+1}$. The Green's function matrix for disordered crystal, $\mathbf{G}(i,j;E)$, is defined by,

$$\mathbf{G}(i,j;E) = \begin{pmatrix} G_{11}^{AA\uparrow\uparrow}(i,j;E) & G_{12}^{AA\uparrow\downarrow}(i,j;E) \\ G_{21}^{AA\downarrow\uparrow}(i,j;E) & G_{22}^{AA\downarrow\downarrow}(i,j;E) \\ G_{11}^{BA\uparrow\uparrow}(i,j;E) & G_{12}^{BA\uparrow\downarrow}(i,j;E) \\ G_{21}^{BA\downarrow\uparrow}(i,j;E) & G_{22}^{BA\downarrow\downarrow}(i,j;E) \end{pmatrix} \begin{pmatrix} G_{11}^{AB\uparrow\uparrow}(i,j;E) & G_{12}^{AB\uparrow\downarrow}(i,j;E) \\ G_{21}^{AB\downarrow\uparrow}(i,j;E) & G_{22}^{AB\downarrow\downarrow}(i,j;E) \\ G_{11}^{BB\uparrow\uparrow}(i,j;E) & G_{12}^{BB\uparrow\downarrow}(i,j;E) \\ G_{21}^{BB\downarrow\uparrow}(i,j;E) & G_{22}^{BB\downarrow\downarrow}(i,j;E) \end{pmatrix}. \tag{13}$$

Equation (2) can be written as,

$$\mathbf{G}(i,j;E) = \mathbf{G}^0(i,j;E) + \sum_{l\acute{l}} \mathbf{G}^0(i,l;E)\mathbf{V}_{l\acute{l}}\mathbf{G}(\acute{l},j;E), \tag{14}$$

where the random potential matrix, $\mathbf{V}_{l\acute{l}}$, is defined by,

$$\mathbf{V}_{l\acute{l}} = \begin{pmatrix} \varepsilon_l\delta_{l\acute{l}} - \sum_{\acute{l}} U_{\acute{l}\acute{l}}n_{\acute{l}\downarrow} & \delta\Delta_l^{\parallel}\delta_{l\acute{l}} + \delta\Delta_{l\acute{l}}^{\perp} \\ \delta\Delta_l^{\parallel}\delta_{l\acute{l}} + \delta\Delta_{l\acute{l}}^{\perp} & -(\varepsilon_l\delta_{l\acute{l}} - \sum_{\acute{l}} U_{\acute{l}\acute{l}}n_{\acute{l}\uparrow}) \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ \varepsilon_l\delta_{l\acute{l}} - \sum_{\acute{l}} U_{\acute{l}\acute{l}}n_{\acute{l}\downarrow} & \delta\Delta_l^{\parallel}\delta_{l\acute{l}} + \delta\Delta_{l\acute{l}}^{\perp} \\ \delta\Delta_l^{\parallel}\delta_{l\acute{l}} + \delta\Delta_{l\acute{l}}^{\perp} & -(\varepsilon_l\delta_{l\acute{l}} - \sum_{\acute{l}} U_{\acute{l}\acute{l}}n_{\acute{l}\uparrow}) \end{pmatrix}, \tag{15}$$

and the clean system Green function, $\mathbf{G}^0(i,j;E)$, is given by,

$$\mathbf{G}^0(i,j;E) = \frac{2}{N}\sum_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_{ij}} \times \begin{pmatrix} E+\mu+\epsilon_{\mathbf{k}}^{\perp} & \Delta^0(\mathbf{k}) & \epsilon_{\mathbf{k}} & 0 \\ \Delta^0(\mathbf{k}) & E-\mu-\epsilon_{\mathbf{k}}^{\perp} & 0 & -\epsilon_{\mathbf{k}} \\ \epsilon_{\mathbf{k}}^* & 0 & E+\mu+\epsilon_{\mathbf{k}}^{\perp} & \Delta^0(\mathbf{k}) \\ 0 & -\epsilon_{\mathbf{k}}^* & \Delta^0(\mathbf{k}) & E-\mu-\epsilon_{\mathbf{k}}^{\perp} \end{pmatrix}^{-1}, \tag{16}$$

where $\epsilon_{\mathbf{k}} = -\frac{2}{N}\sum_{ij} t_{ij}\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_{ij}}$ is the band structure and $\Delta^0(\mathbf{k}) = \Delta^{0\parallel} + \Delta^{0\perp}(\mathbf{k})$ is the Fourier transform of the clean system order parameter. We choose basic vectors as (figure 1),

$$\mathbf{a}_{01} = \frac{a_0}{2}\mathbf{e}_1 - \frac{\sqrt{3}a_0}{2}\mathbf{e}_2, \qquad \mathbf{a}_{02} = \frac{a_0}{2}\mathbf{e}_1 + \frac{\sqrt{3}a_0}{2}\mathbf{e}_2, \qquad \mathbf{a}_{03} = -(\mathbf{a}_{01}+\mathbf{a}_{02}), \tag{17}$$

$$\mathbf{a}_1 = a\mathbf{e}_1, \qquad \mathbf{a}_2 = -\frac{\sqrt{3}a}{2}\mathbf{e}_1 + \frac{a}{2}\mathbf{e}_2, \qquad \mathbf{a}_3 = c\mathbf{e}_3, \tag{18}$$

where $a_0 = \frac{a}{\sqrt{3}}$. In our numerical calculations, hopping to the first nearest neighbors' intra a B_2 plane and inter B_2 planes is considered, and we neglected other hopping terms, so

$$\epsilon_{\mathbf{k}}^{\parallel\pm} = \epsilon_{\mathbf{k}}^{\pm} = \pm t^{\parallel}\sqrt{1+4\left[\cos\left(\frac{\sqrt{3}k_xa}{2}\right)+\cos\left(\frac{k_ya}{2}\right)\right]\cos\left(\frac{k_ya}{2}\right)}, \tag{19}$$

$$\epsilon_{\mathbf{k}}^{\perp} = 2t^{\perp}\cos(ck_z). \tag{20}$$

Here $t^{\parallel} = t_{\langle ij\rangle}^{AB} = t_{\langle ij\rangle}^{BA}$ and $t^{\perp} = t_{\langle ij\rangle}^{AA} = t_{\langle ij\rangle}^{BB}$ are hopping integrals intra a B_2 plane and inter B_2 planes, respectively. Here we do not consider randomness in U_{ij}, hence the interaction potential is chosen to be $U_i^{\parallel} = 2.5t$, where $t^{\parallel} = t = 1.6$ eV and $t^{\perp} = 0.96$ eV. Also, for comparison of our results with experimental data, we set the impurity scattering strength, $\delta = 4.5t$, and chemical potential, $\mu = -0.47t$.

The Dyson equation corresponding to equation (14) for the average Green's function, $\bar{\mathbf{G}}(i,j;E)$, is given by,

$$\bar{\mathbf{G}}(i,j;E) = \mathbf{G}^0(i,j;E) + \sum_{l\acute{l}} \mathbf{G}^0(i,l;E)\boldsymbol{\Sigma}(l,\acute{l},E)\bar{\mathbf{G}}(\acute{l},j;E), \tag{21}$$

where the self-energy, $\boldsymbol{\Sigma}(l,\acute{l},E)$, is defined by,

$$\sum_{\acute{l}}\langle\mathbf{V}_{l\acute{l}}\mathbf{G}(\acute{l},j;E)\rangle = \sum_{\acute{l}}\boldsymbol{\Sigma}(l,\acute{l},E)\bar{\mathbf{G}}(\acute{l},j;E). \tag{22}$$

The Fourier transformation of equation (21) leads to the following relation for the average Green's function matrix, $\bar{\mathbf{G}}(i,j;E)$:

$$\bar{\mathbf{G}}(i,j;E) = \frac{2}{N}\sum_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_{ij}} \times \begin{pmatrix} E+\mu+\epsilon_{\mathbf{k}}^{\perp}-\Sigma_{11}(\mathbf{k},E) & \Delta^0(\mathbf{k})-\Sigma_{12}(\mathbf{k},E) \\ \Delta^0(\mathbf{k})-\Sigma_{21}(\mathbf{k},E) & E-\mu-\epsilon_{\mathbf{k}}^{\perp}-\Sigma_{22}(\mathbf{k},E) \\ \epsilon_{\mathbf{k}}^* & 0 \\ 0 & -\epsilon_{\mathbf{k}}^* \end{pmatrix} \begin{pmatrix} \epsilon_{\mathbf{k}} & 0 \\ 0 & -\epsilon_{\mathbf{k}} \\ E+\mu+\epsilon_{\mathbf{k}}^{\perp}-\Sigma_{33}(\mathbf{k},E) & \Delta^0(\mathbf{k})-\Sigma_{34}(\mathbf{k},E) \\ \Delta^0(\mathbf{k})-\Sigma_{43}(\mathbf{k},E) & E-\mu-\epsilon_{\mathbf{k}}^{\perp}-\Sigma_{44}(\mathbf{k},E) \end{pmatrix}^{-1}. \tag{23}$$

Equations (10)–(23) should be solved to determine the average Green's function, $\bar{\mathbf{G}}(i,j;E)$. In general, there is no analytical solution for such random systems, hence it should be solved approximately. There are many approximations such as the self-consistent Born approximation or Abrikosov–Gorkov theory, which is valid for weak scattering ($\delta \ll$ bandwidth) and all impurity concentrations [20], the self-consistent T-matrix approximation, which is limited to the case of low impurity concentrations [21], and the coherent potential approximation (CPA), which is valid for all impurity concentrations and impurity strengths [20]. We use the coherent potential approximation (CPA) to obtain the average Green's function matrix, $\bar{\mathbf{G}}(i,j;E)$, and T_c. In the next section, we derive a set of equations for the calculation of T_c in the CPA formalism.

3. Calculation of T_c in the CPA formalism

To investigate the effects of impurities, identified by their strength δ and concentration c, on the critical temperature, T_c, of MgB_2 superconductor, we used the CPA. In the CPA formalism, inter-site correlations are neglected and each lattice site is replaced by an effective site, except for one, which is called the impurity site and is denoted by i. So the self-energy is local and takes the same value for all sites, $\mathbf{\Sigma}(i, j, E) = \mathbf{\Sigma}(E)\delta_{ij}$; also, in the random potential, we consider just the local random terms, $\delta\Delta_{ij} = \delta\Delta_i^{\parallel}\delta_{ij}$. Hence equations (22) and (23) are reduced to [21]

$$\langle \mathbf{V}_i \mathbf{G}^{\mathrm{imp}}(i, i; E)\rangle = \mathbf{\Sigma}(E)\bar{\mathbf{G}}(i, i; E), \tag{24}$$

and

$$\bar{\mathbf{G}}(i, j; E) = \frac{2}{N}\sum_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_{ij}} \times \begin{pmatrix} E+\mu+\epsilon_{\mathbf{k}}^{\perp}-\Sigma_{11}(E) & \Delta^0(\mathbf{k})-\Sigma_{12}(E) \\ \Delta^0(\mathbf{k})-\Sigma_{21}(E) & E-\mu-\epsilon_{\mathbf{k}}^{\perp}-\Sigma_{22}(E) \\ \epsilon_{\mathbf{k}}^{*} & 0 \\ 0 & -\epsilon_{\mathbf{k}}^{*} \end{pmatrix} \begin{pmatrix} \epsilon_{\mathbf{k}} & 0 \\ 0 & -\epsilon_{\mathbf{k}} \\ E+\mu+\epsilon_{\mathbf{k}}^{\perp}-\Sigma_{33}(E) & \Delta^0(\mathbf{k})-\Sigma_{34}(E) \\ \Delta^0(\mathbf{k})-\Sigma_{43}(E) & E-\mu-\epsilon_{\mathbf{k}}^{\perp}-\Sigma_{44}(E) \end{pmatrix}^{-1}, \tag{25}$$

respectively, where the impurity Green's function, $\mathbf{G}^{\mathrm{imp}}(i, i; E)$, is related to the averaged Green's function, $\bar{\mathbf{G}}(i, i, ; E)$, by [21, 22]

$$\mathbf{G}^{\mathrm{imp}}(i, i; E) = \bar{\mathbf{G}}(i, i; E) + \bar{\mathbf{G}}(i, i; E)(\mathbf{V}_i - \mathbf{\Sigma}(E))\mathbf{G}^{\mathrm{imp}}(i, i; E). \tag{26}$$

Also, the random potential in equation (15) is reduced to

$$\mathbf{V}_i = \begin{pmatrix} \varepsilon_i - U_i^{\parallel} n_{i\downarrow} & \delta\Delta_i^{\parallel} & 0 & 0 \\ \delta\Delta_i^{\parallel} & -(\varepsilon_i - U_i^{\parallel} n_{i\uparrow}) & 0 & 0 \\ 0 & 0 & \varepsilon_i - U_i^{\parallel} n_{i\downarrow} & \delta\Delta_i^{\parallel} \\ 0 & 0 & \delta\Delta_i^{\parallel} & -(\varepsilon_i - U_i^{\parallel} n_{i\uparrow}) \end{pmatrix}. \tag{27}$$

The new average Green's function, $\bar{\mathbf{G}}(i, i, ; E)$, is given by taking the average over all possible impurity configurations:

$$\bar{\mathbf{G}}(i, i; E) = \langle \mathbf{G}^{\mathrm{imp}}(i, i; E)\rangle. \tag{28}$$

Since site i can pertain to non-equivalent sub-sites A and B, four possible configurations at this site are: boron–boron (both sub-sites A and B of site i are boron atoms); boron–impurity (sub-site A is a boron atom, while sub-site B is an impurity); impurity–boron (sub-site A is an impurity atom, while sub-site B is a boron atom); and impurity–impurity (both sub-sites A and B of site i are impurity atoms). The probability of these configurations are $P_1 = (1-c)^2$, $P_2 = (1-c)c$, $P_3 = c(1-c)$ and $P_4 = c^2$, respectively. The average intra-plane order parameter is calculated from

$$\bar{\Delta}_i^{\parallel} = \sum_{\gamma=1}^{4} P_\gamma \Delta_i^{\parallel\gamma}. \tag{29}$$

Equations (24)–(29) should be solved self-consistently to provide the average Green's function, $\bar{\mathbf{G}}(i, i, ; E)$, in the CPA formalism. We continue our discussions by deriving a set of equations to obtain the critical temperature in the CPA formalism. At T_c both the local and average intra B_2 plane order parameters, $\Delta_i^{\parallel}$ and $\bar{\Delta}^{\parallel}$, go to zero, and the spatial deviation of the local order parameter, $\delta\Delta_i^{\parallel}$, with respect to the averaged order parameter, $\bar{\Delta}^{\parallel}$, is negligible, so

$$\Delta_i^{\parallel} \approx \bar{\Delta}^{\parallel}. \tag{30}$$

By inserting equation (30) into equation (24) we found that [10]

$$\bar{\Delta}^{\parallel} = \Sigma_{12}(E) = \Sigma_{34}(E). \tag{31}$$

By using equation (30) and the gap equation (10), for the average order parameter, $\bar{\Delta}^{\parallel}$, at T_c we obtain,

$$-\frac{U_i^{\parallel}}{\pi}\int_{-\infty}^{+\infty} \mathrm{d}E f(E)\,\mathrm{Im}\left[\int_{-\infty}^{+\infty} \mathrm{d}\epsilon N^{0\parallel}(\epsilon)\int_{-\infty}^{+\infty} \mathrm{d}\acute{\epsilon} N^{0\perp}(\acute{\epsilon}) \times \bar{G}_{12}(i, i; E+\mathrm{i}0^+)\right] = 1, \tag{32}$$

where $N^{0\parallel}(\epsilon)$ and $N^{0\perp}(\acute{\epsilon})$ represent the clean system density of states and are defined by

$$N^{0\parallel}(\epsilon) = \frac{2}{N^{\parallel}}\sum_{\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k}}), \tag{33}$$

$$N^{0\perp}(\acute{\epsilon}) = \frac{1}{N^{\perp}}\sum_{\mathbf{k}} \delta(\acute{\epsilon} - \epsilon_{\mathbf{k}}^{\perp}). \tag{34}$$

In equation (32), $\bar{G}_{12}(i, i; E+\mathrm{i}0^+)$ is

$$\bar{G}_{12}(i, i; E+\mathrm{i}0^+) = \frac{\zeta(\epsilon, \acute{\epsilon}; E+\mathrm{i}0^+)}{\xi(\epsilon, \acute{\epsilon}; E+\mathrm{i}0^+)}, \tag{35}$$

where

$$\zeta(\epsilon, \acute{\epsilon}; E+\mathrm{i}0^+) = -\epsilon^2 + [(E+\mathrm{i}0^+) + \mu + \acute{\epsilon} - \Sigma_{33}(E+\mathrm{i}0^+)][(E+\mathrm{i}0^+) - \mu - \acute{\epsilon} - \Sigma_{44}(E+\mathrm{i}0^+)], \tag{36}$$

and

$$\begin{aligned}\xi(\epsilon, \acute{\epsilon}; E+\mathrm{i}0^+) = \epsilon^4 - \epsilon^2\{&[(E+\mathrm{i}0^+) + \mu + \acute{\epsilon} - \Sigma_{11}(E+\mathrm{i}0^+)][(E+\mathrm{i}0^+) + \mu + \acute{\epsilon} - \Sigma_{33}(E+\mathrm{i}0^+)] \\ &+ [(E+\mathrm{i}0^+) - \mu - \acute{\epsilon} - \Sigma_{22}(E+\mathrm{i}0^+)][(E+\mathrm{i}0^+) - \mu - \acute{\epsilon} - \Sigma_{44}(E+\mathrm{i}0^+)]\} \\ &+ [(E+\mathrm{i}0^+) + \mu + \acute{\epsilon} - \Sigma_{11}(E+\mathrm{i}0^+)][(E+\mathrm{i}0^+) - \mu - \acute{\epsilon} - \Sigma_{22}(E+\mathrm{i}0^+)] \\ &\times [(E+\mathrm{i}0^+) + \mu + \acute{\epsilon} - \Sigma_{33}(E+\mathrm{i}0^+)][(E+\mathrm{i}0^+) - \mu - \acute{\epsilon} - \Sigma_{44}(E+\mathrm{i}0^+)].\end{aligned} \tag{37}$$

Equations (30) and (31) and equations (24)–(29) should be solved self-consistently to calculate $\Sigma_{11}(E+\mathrm{i}0^+)$, $\Sigma_{22}(E+\mathrm{i}0^+)$, $\Sigma_{33}(E+\mathrm{i}0^+)$ and $\Sigma_{44}(E+\mathrm{i}0^+)$. Then these self-energies should be inserted into equation (32) to obtain the critical temperature, T_c.

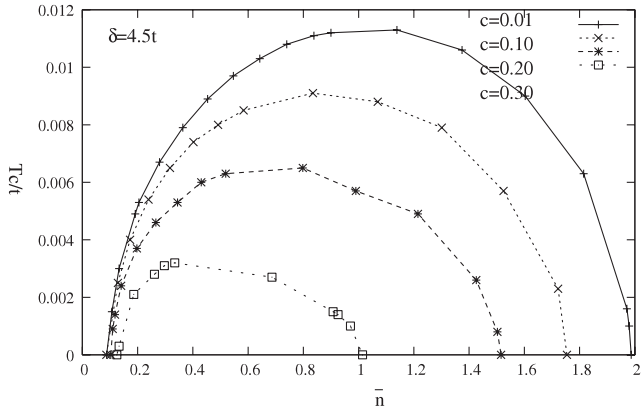

Figure 2. T_c/t in terms of the average band filling, $\bar{n}$, for different impurity concentrations, c, where $\delta = 4.5t$ bandwidth.

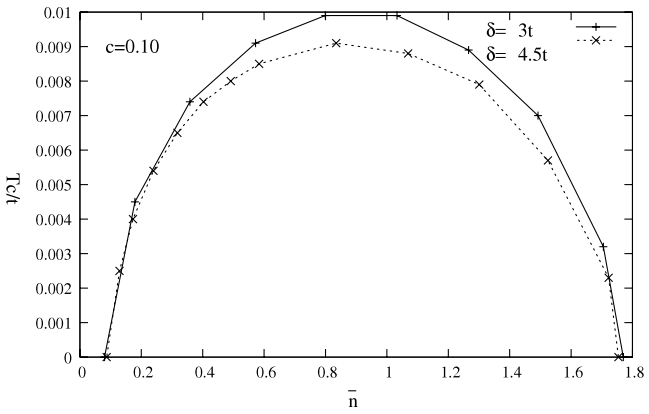

Figure 3. T_c/t in terms of the average band filling, $\bar{n}$, for different values of the scattering strength, δ.

4. Results and discussions

We have investigated the reduction of the critical temperature, T_c, of MgB_2 in terms of non-magnetic impurity doping for different impurity concentrations, c, and different values of scattering strength, δ. To find the role of such impurities on the reduction of T_c, we have calculated T_c by varying the impurity concentration c, impurity strength δ, and chemical potential μ. Figure 2 illustrates T_c/t in terms of the average band filling, $\bar{n}$, at fixed impurity strength, $\delta = 4.5t$, for different impurity concentrations, $c = 0.01$, 0.10, 0.20 and 0.30, where T_c is calculated from equation (32); we found that, by increasing the impurity concentration, the critical temperature is reduced and, for some average band filling, there is no superconductivity state. To consider the effect of the scattering strength on T_c, we have plotted T_c/t in terms of the average band filling for a fixed impurity concentration and for different scattering strengths.

Figures 3–5 show T_c/t in terms of the average band filling for a fixed impurity concentration and for different values of the scattering strength, $\delta = 3t$ and $\delta = 4.5t$; for all these impurity concentrations, T_c decreased. Figure 6 illustrates that, by increasing the impurity strength and the impurity concentrations, T_c decreased again. To compare

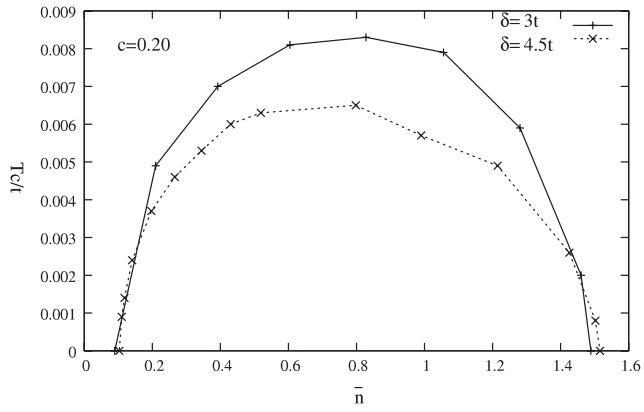

Figure 4. T_c/t in terms of the average band filling, $\bar{n}$, for different values of the scattering strength, δ.

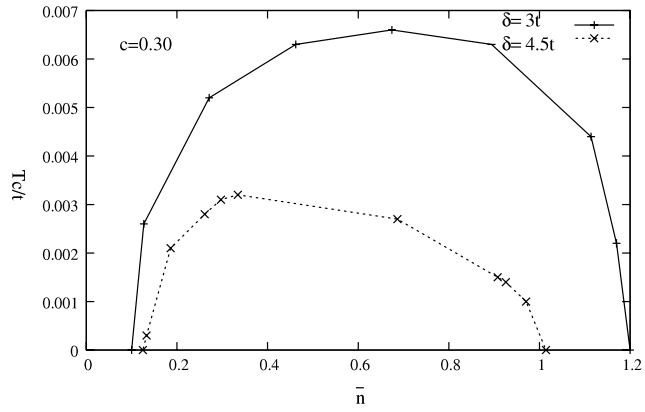

Figure 5. T_c/t in terms of the average band filling, $\bar{n}$, for different values of the scattering strength, δ.

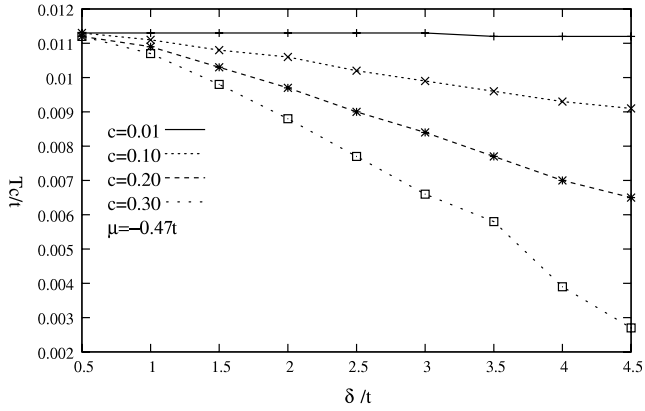

Figure 6. T_c/t in terms of the scattering strength, δ/t, for different values of impurity concentrations, c.

our results with experimental data, we calculated T_c in terms of the impurity concentration at a fixed impurity strength and also a fixed chemical potential; we found that, just for $\delta = 4.5t$ and $\mu = -0.47t$, our results are in agreement with the reported experimental results [17, 18]. Now we use these parameters, $\delta = 4.5t$ and $\mu = -0.47t$, to calculate T_c in terms of the impurity concentrations, c. Figure 7

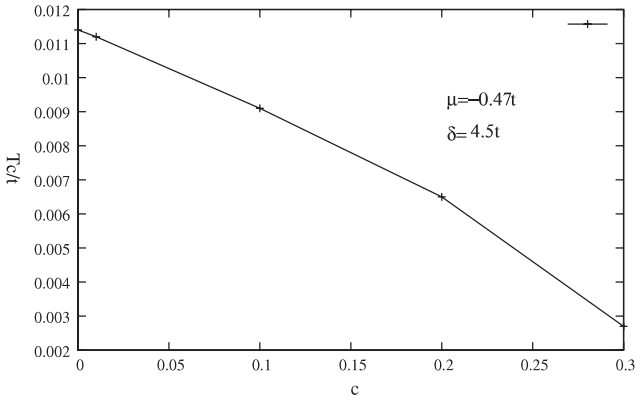

Figure 7. T_c/t in terms of impurity concentrations, c, where $\delta = 4.5t$ bandwidth; shown experimentally in [17, 18].

shows T_c/t in terms of the impurity concentrations for a fixed chemical potential, $\mu = -0.47t$, and a fixed impurity strength, $\delta = 4.5t$, T_c is reduced linearly by increasing the impurity concentration, where it is compatible with the experimental results reported in [17, 18] where they found that the superconducting transition temperature decreases monotonically with increasing carbon content in the full range of substitution that was investigated.

5. Conclusion

In conclusion, we have investigated the reduction of the critical temperature T_c of MgB_2 superconductor in terms of the non-magnetic impurity doping. Three cases are considered: first, at a fixed scattering strength δ, T_c is calculated for different impurity concentrations, c. Second, at fixed impurity concentrations c, T_c is calculated for different scattering strengths, δ. Finally, we have investigated the behavior of T_c in terms of c for a fixed chemical potential. We found that, by increasing δ and c, the critical temperature decreased and, for some average band fillings, superconductivity disappears. By comparing our results with experimental data, we found that, just for $\delta = 4.5t$ and $\mu = -0.47t$, T_c reduces approximately linearly in terms of the impurity concentration, c.

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