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Analysis of Superconducting Microstructures: Formulation

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SYNOPSIS

Numerical methods for the analysis of the proximity effect in superconducting microstructures in the dirty limit are formulated on the basis of the finite element method. One- and two-dimensional cases are considered and third order Hermite shape functions are used. The results are also applicable to investigations of electronic states in semiconductor superlattice structures.

I. INTRODUCTION

Microstructures including superconducting materials have a possibility to show novel properties quite different from those of bulk solids. These properties are also important in relation to applications of superconducting materials to electronic devices.[1]

In order to analyze the critical parameters of microstructures including superconductors, it is necessary to determine the behavior of the order parameter or the pair potential. Since the superconducting proximity effect[2,3] plays a very important role in these structures, we have to take the geometry of the system properly into account in such an analysis.

In this paper, we consider the system where the mean free path of electrons is smaller than other characteristic lengths or the case in the dirty limit. This is one of important cases in real structures and also greatly simplifies the theoretical treatment of the proximity effect.

The proximity effect in the dirty limit has been first formulated by de Gennes[2] and extended to general inhomogeneous cases recently.[3]

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In early investigations,[4] the results are limited to simple one-dimensional cases where the analytical treatment is possible at least up to some stage. In order to analyze the geometrical effect, it may be necessary to consider the case of two or more space dimensions. We are thus forced to employ some numerical method even in the simplest cases.

As a numerical method, the finite element method may be useful to take the effect of geometry into account. The purpose of this paper is to give a formulation of numerical analyses of the superconducting proximity effect based on this method.

We here note that the fundamental equation for electrons in the semiconductor superlattices takes a similar form in the effective mass approximation. In relation to applications to electronic devices, quantum states in this system also requires considerations of geometrical effects. The result will also be useful in investigating electronic states in semiconductor superlattices.

II. FUNDAMENTAL EQUATIONS

The essential part of the analysis of the proximity effect[3] is to obtain the eigenfunctions $\phi_n(\mathbf{r})$ of the operator $\hat{L}$ defined by

$$\hat{L} = -\frac{\hbar}{N(\mathbf{r})}(\nabla_{\mathbf{r}} - a\mathbf{A}(\mathbf{r})) \cdot \mathsf{D}(\mathbf{r})N(\mathbf{r})(\nabla_{\mathbf{r}} - a\mathbf{A}(\mathbf{r})), \tag{2.1}$$

where $\mathsf{D}(\mathbf{r})$ is the diffusion tensor, $N(\mathbf{r})$, the local density of states, $\mathbf{A}(\mathbf{r})$, the vector potential, and

$$a = 2ie/\hbar c. \tag{2.2}$$

We denote the eigenvalues of $\hat{L}$ by E_n ;

$$[\hat{L} - E_n]\phi_n(\mathbf{r}) = 0. \tag{2.3}$$

The boundary conditions are

$$\phi_n(\mathbf{r}) = \text{continuous} \tag{2.4}$$

and

$$\mathbf{n} \cdot N(\mathbf{r})\mathsf{D}(\mathbf{r})(\nabla_{\mathbf{r}} - a\mathbf{A}(\mathbf{r}))\phi_n(\mathbf{r}) = \begin{cases} \text{continuous (at interfaces)}, \\ 0 \text{ (at surfaces)}, \end{cases} \tag{2.5}$$

$\mathbf{n}$ being the unit vector normal to interfaces or surfaces.

It is to be noted that the kinetic energy of an electron in semiconductor superlattices is similar to the operator $\hat{L}$ with $\mathbf{A} = 0$ in the effective mass approximation.

We define the inner product of functions Ψ and Φ as

$$(\Psi, \Phi) = \int d\mathbf{r} N(\mathbf{r}) \Psi(\mathbf{r}) \Phi(\mathbf{r}). \tag{2.6}$$

The operator $\hat{L}$ then becomes Hermitian and we assume that the eigenfunctions of the operator $\hat{L}$ form a complete orthogonal set.

The critical parameters are determined by the condition

$$\det \mid C_{nn'} \mid = 0, \tag{2.7}$$

where

$$C_{nn'} = \delta_{nn'} - \frac{A_n}{[(\phi_n, \phi_n)(\phi_{n'}, \phi_{n'})]^{\frac{1}{2}}} \int d\mathbf{r} N(\mathbf{r}) \phi_n(\mathbf{r}) V(\mathbf{r}) N(\mathbf{r}) \phi_{n'}(\mathbf{r}), \tag{2.8}$$

$$A_n = \ln(1.13 \frac{(k_B \Theta_D + E_n)}{k_B T}) + \psi(\frac{1}{2}) - \psi(\frac{1}{2} + \frac{E_n}{4\pi k_B T}), \tag{2.9}$$

$V(\mathbf{r})$ is the (attractive) interaction between electrons, $\psi(x)$ is the digamma function, and Θ_D is the Debye temperature.

In the calculation of A_n we have followed the standard cutoff procedure[2,5] of the summation over the Matsubara frequency at the Debye temperature and implicitly assumed that the latter is almost independent of the constituent materials.

We normalize the variables $N(\mathbf{r})$, $\mathrm{D}(\mathbf{r})$, and $\mathbf{r}$ by their typical values N_0, D_0, and L_0 and rewrite the equation as

$$(\mathcal{L} - \varepsilon_n)\, \phi(\rho) = 0. \tag{2.10}$$

Here

$$\rho = \mathbf{r}/L_0, \tag{2.11}$$

$$\mathcal{L} = -\frac{1}{\nu(\rho)} (\nabla_\rho - \alpha) \cdot \nu(\rho) \delta(\rho) (\nabla_\rho - \alpha), \tag{2.12}$$

$$\nu = N/N_0, \tag{2.13}$$

$$\delta = \mathrm{D}/D_0, \tag{2.14}$$

$$\alpha = L_0(2ie/\hbar c), \tag{2.15}$$

$$\varepsilon_n = E_n / \left(\frac{\hbar D_0}{L_0^2}\right). \tag{2.16}$$

As N_0 and D_0 we take the values of N and D in the superconducting domain and, as L_0, the characteristic scale of length of the system. We denote the components of ρ by x, y, and z, as $\rho = (x, y, z)$, and ∇_ρ simply by ∇. We assume that D reduces to a scalar D in what follows.

III. ONE-DIMENSIONAL ANALYSIS

A. Analytical Treatment

When the structure of the system is simple, analytical treatment is possible up to some stage of the analysis. As one of such examples, we here consider the case of a bilayer composed of the normal and superconducting parts without the magnetic field. Both parts are uniform and characterized by thicknesses d_N and d_S, the density of states N_S and N_N, the diffusion coefficient D_S and D_N, and the effective interaction between electrons V_S and V_N: Parameters of superconducting and normal parts are specified by subscripts S and N, respectively. We define L_0, N_0, D_0, ν, δ by

$$L_0 = d = d_S + d_N, \tag{3.1}$$
$$N_0 = N_S, \tag{3.2}$$
$$D_0 = D_S, \tag{3.3}$$
$$\nu = N_N/N_S, \tag{3.4}$$
$$\delta = D_N/D_S, \tag{3.5}$$

and take the coordinate x so that $(0, d_N/d)$ is a uniform normal layer characterized by ν and δ, and $(d_N/d, 1)$, a uniform superconducting layer.

In the normal and super parts, the eigenfunction is given respectively by

$$a_N \cos(k_N x), \tag{3.6}$$
$$a_S \cos[k_S(1-x)], \tag{3.7}$$

with

$$\varepsilon_n/\delta = k_N^2, \tag{3.8}$$
$$k_S = \delta^{1/2} k_N. \tag{3.9}$$

The boundary conditions at $x = x_1 = d_N/d$ are

$$a_N \cos(k_N x_1) = a_S \cos[k_S(1-x_1)], \tag{3.10}$$
$$\nu\delta a_N k_N \sin(k_N x_1) = -a_S k_S \sin[k_S(1-x_1)], \tag{3.11}$$

or

$$\tan k + \nu^{-1}\delta^{-1/2} \tan\left[\delta^{1/2} k(1-x_1)/x_1\right] = 0, \tag{3.12}$$

where

$$k = k_N x_1. \tag{3.13}$$

The eigenfunction is normalized so that

$$\nu \int_0^{x_1} dx a_N^2 \cos^2(k_N x) + \int_{x_1}^1 dx a_S^2 \cos^2[k_S(1-x)] = 1, \tag{3.14}$$

or

$$a_N^{-2} = \frac{\nu x_1}{4k}[2k + \sin 2k] + \frac{x_1}{4k\delta^{1/2}}\left[2k\delta^{1/2}\frac{1-x_1}{x_1} + \sin(2k\delta^{1/2}\frac{1-x_1}{x_1})\right]\frac{\cos^2 k}{\cos^2(k\delta^{1/2}(1-x_1)/x_1)}. \tag{3.15}$$

The matrix element included in the equation to determine the critical temperature is given as

$$\begin{aligned}
&\int_0^1 dx\, N(x)\phi(x)N(x)V(x)\phi'(x) \\
&= N_0^2 V_0 \left[\nu^2 v a_N a'_N \int_0^{x_1} dx \cos(k_N x)\cos(k'_N x) + a_S a'_S \int_0^{1-x_1} dx \cos(k_S x)\cos(k'_S x)\right] \\
&= \frac{N_0^2 V_0}{2}\Big(\nu^2 v a_N a'_N \left[\frac{\sin[(k_N + k'_N)x_1]}{(k_N + k'_N)} + \frac{\sin[(k_N - k'_N)x_1]}{(k_N - k'_N)}\right] \\
&\quad + a_S a'_S \left[\frac{\sin[(k_S + k'_S)(1-x_1)]}{(k_S + k'_S)} + \frac{\sin[(k_S - k'_S)(1-x_1)]}{(k_S - k'_S)}\right]\Big),
\end{aligned} \tag{3.16}$$

where

$$v = V_N/V_S. \tag{3.17}$$

In eq.(3.16) we take the appropriate limit when the denominator vanishes.

As shown above, the matrix element $C_{nn'}$ are obtained analytically for this simple case. Equation (2.7) itself, however, needs numerical computations.

B. Hermite Shape Functions

In order to analyze general cases, it is necessary to use numerical methods to solve eq.(2.7) even in one dimension. We here adopt the finite element method as one of such procedures.

Noting the boundary conditions for the derivative, we use the Hermite interpolations with the first order derivatives as the shape functions for each element. In the element (x_1, x_2), these functions are given by

$$N_1 = 2s^3 - 3s^2 + 1, \tag{3.18}$$

$$\tilde{N}_{1x} = L(s^3 - 2s^2 + s), \tag{3.19}$$

$$N_2 = -2s^3 + 3s^2, \tag{3.20}$$

$$\tilde{N}_{2x} = L(s^3 - s^2), \tag{3.21}$$

where $L = x_2 - x_1$ and $s = (x - x_1)/L$. They are characterized by their values and derivatives at boundaries as shown in the next table;

	$\phi(x_1)$	$\phi'(x_1)$	$\phi(x_2)$	$\phi'(x_2)$
N_1	1	0	0	0
$\tilde{N}_{1x}$	0	1	0	0
N_2	0	0	1	0
$\tilde{N}_{2x}$	0	0	0	1

As shape functions we adopt N_1, N_2, N_{1x}, and N_{2x} where the latter two are defined by

$$N_{1x} = \frac{\tilde{N}_{1x}}{\nu(x_1)\delta(x_1)}, \tag{3.22}$$

$$N_{2x} = \frac{\tilde{N}_{2x}}{\nu(x_2)\delta(x_2)}. \tag{3.23}$$

When ν and δ have discontinuities at boundaries, values in these expressions are taken to be the limiting values from inside of each element.

We divide the whole domain into n elements and expand the solution of our equation by shape functions in each element specified by the superscript (l) as

$$\phi = \sum_{l=1}^{n} \left[N_1^{(l)} N_{1x}^{(l)} N_2^{(l)} N_{2x}^{(l)} \right] \begin{bmatrix} \phi_1^{(l)} \\ \phi_{1x}^{(l)} \\ \phi_2^{(l)} \\ \phi_{2x}^{(l)} \end{bmatrix}. \tag{3.24}$$

When the element $(l-1)$ is placed to the left of the element (l), the values of the solution and its derivative at the right-hand side of the element $(l-1)$ and those at the left-hand side of the element (l), referring to the same node, are not independent. This relation is generally expressed by the 2×2 interface matrix $t^{(l)}$ $(l \geq 2)$ as

$$\begin{bmatrix} \phi_1^{(l)} \\ \phi_{1x}^{(l)} \end{bmatrix} = \begin{bmatrix} t_{11}^{(l)}, & t_{12}^{(l)} \\ t_{21}^{(l)}, & t_{22}^{(l)} \end{bmatrix} \begin{bmatrix} \phi_2^{(l-1)} \\ \phi_{2x}^{(l-1)} \end{bmatrix}. \tag{3.25}$$

In the case of the Schrödinger equation where ν and δ are constant throughout the whole space, the matrix $t^{(l)}$ reduces to the unit matrix. In the general case of position dependent ν or δ, however, the derivative of ϕ itself is not continuous at discontinuities of these functions and $t^{(l)}$ is different from the unit matrix.

In our case, ϕ and $\nu\delta(d/dx)\phi$ are continuous. Therefore, when we use the shape functions defined above, *the matrix $t^{(l)}$ is still the unit matrix.* It is thus unnecessary to take the boundary conditions between elements into account explicitly.

We also note that, with magnetic field, the interface matrix takes the form

$$\begin{bmatrix} t_{11}^{(l)} = 1, & t_{12}^{(l)} = 0 \\ t_{21}^{(l)} = *, & t_{22}^{(l)} = 1 \end{bmatrix} \begin{bmatrix} \phi_2^{(l-1)} \\ \phi_{2x}^{(l-1)} \end{bmatrix} \tag{3.26}$$

with nonzero element $t_{21}^{(l)} = *$ when $\nu\delta$ has discontinuities.

C. Galerkin Equation

The inner product of functions Ψ and Φ is defined by the integral over the domain of interest with the weighting function $\nu(x)$:

$$(\Psi, \Phi) = \int dx \nu(x) \Psi(x) \Phi(x). \tag{3.27}$$

We rewrite our equation (2.10) into the weak form by taking the inner product with the function ψ which has the same form as the solution (3.24);

$$(\psi, (\mathcal{L} - \varepsilon)\, \phi) = 0, \tag{3.28}$$

where

$$\psi = \sum_{l=1}^{n} \begin{bmatrix} \psi_1^{(l)} \psi_{1x}^{(l)} \psi_2^{(l)} \psi_{2x}^{(l)} \end{bmatrix} \begin{bmatrix} N_1^{(l)} \\ N_{1x}^{(l)} \\ N_2^{(l)} \\ N_{2x}^{(l)} \end{bmatrix}. \tag{3.29}$$

We thus have

$$\int_D dx\, \nu \sum_{l,m=1}^{n} \begin{bmatrix} \psi_1^{(l)} \psi_{1x}^{(l)} \psi_2^{(l)} \psi_{2x}^{(l)} \end{bmatrix} \begin{bmatrix} N_1^{(l)} \\ N_{1x}^{(l)} \\ N_2^{(l)} \\ N_{2x}^{(l)} \end{bmatrix} (\mathcal{L} - \varepsilon) \begin{bmatrix} N_1^{(m)} N_{1x}^{(m)} N_2^{(m)} N_{2x}^{(m)} \end{bmatrix} \begin{bmatrix} \phi_1^{(m)} \\ \phi_{1x}^{(m)} \\ \phi_2^{(m)} \\ \phi_{2x}^{(m)} \end{bmatrix}$$

$$= \sum_{l=1}^{n} \begin{bmatrix} \psi_1^{(l)} \psi_{1x}^{(l)} \psi_2^{(l)} \psi_{2x}^{(l)} \end{bmatrix} \begin{bmatrix} F_{ij}^{(l)} \end{bmatrix} \begin{bmatrix} \phi_1^{(l)} \\ \phi_{1x}^{(l)} \\ \phi_2^{(l)} \\ \phi_{2x}^{(l)} \end{bmatrix} = 0. \tag{3.30}$$

Here $\left[F_{ij}^{(l)}\right]$ for the element (l) is defined by

$$\left[F_{ij}^{(l)} \right] = \left[K_{ij}^{(l)}\right] - \varepsilon \left[M_{ij}^{(l)}\right] + \left[D_{ij}^{(l)}\right] \tag{3.31}$$

with

$$K_{ij}^{(l)} = \int_{(l)} dx \nu \delta \frac{d}{dx} N_i^{(l)} \frac{d}{dx} N_j^{(l)}, \tag{3.32}$$

$$M_{ij}^{(l)} = \int_{(l)} dx \nu N_i^{(l)} N_j^{(l)}, \tag{3.33}$$

and $[D_{ij}]$ is defined only for the outermost elements as the value at the surface,

$$\left[D_{ij}^{(l)}\right] = \mp \nu \delta N_i \frac{d}{dx} N_j^{(l)}, \tag{3.34}$$

the upper and lower signs corresponding to the right-hand and left-hand surfaces, respectively.

The Galerkin equation is obtained from (3.30) by equating the coefficient of $\psi_i^{(l)}$ at each node to zero, or superposing

$$\left[F_{ij}^{(l)} \right] \begin{bmatrix} \phi_1^{(l)} \\ \phi_{1x}^{(l)} \\ \phi_2^{(l)} \\ \phi_{2x}^{(l)} \end{bmatrix} = 0 \tag{3.35}$$

so as to collect the coefficient for the same node coming from adjacent element.

D. Boundary Conditions

The boundary conditions at surfaces are that the derivative of ϕ vanishes. As a special case of the natural boundary conditions, our Galerkin equations with

$$\left[D_{ij}^{(l)}\right] = 0 \tag{3.36}$$

give solutions satisfying these conditions. We thus discard $\left[D_{ij}^{(l)}\right]$ in our Galerkin equations.

IV. TWO-DIMENSIONAL ANALYSIS

Here we extend our method to the case of two-dimensional structures. As in the one-dimensional case, we assume no magnetic field and confine ourselves within the analysis of the critical temperature.

A. Division into Elements

We first divide the domain of our interest into triangular elements. In this process, we try to keep to conserve as many symmetry properties, such as symmetry axes and mirror planes, of the original domain as possible.

In each triangular element with vertices (in the counterclockwise order) $P_1(x_1, y_1)$, $P_2(x_2, y_2)$, and $P_3(x_3, y_3)$, we take the area coordinates (ξ_1, ξ_2, ξ_3) defined by

$$\xi_1 = \frac{1}{2S}[(x_2y_3 - x_3y_2) + (y_2 - y_3)x - (x_2 - x_3)y], \tag{4.1}$$

$$\xi_2 = \frac{1}{2S}[(x_3y_1 - x_1y_3) + (y_3 - y_1)x - (x_3 - x_1)y], \tag{4.2}$$

$$\xi_3 = 1 - \xi_1 - \xi_2, \tag{4.3}$$

where S is the area of the element.

B. Shape Functions

As in the one-dimensional case, we use the third-order Hermite interpolations as shape functions. Since the third order polynomial in x and y (or ξ_1 and ξ_2) has ten terms, we have ten degrees of freedom.

In two dimensions, each element has lines (sides) in common with adjacent elements, instead of points (nodes) in the one-dimensional case. The boundary conditions are

$$\phi_n(x, y) = \text{continuous} \tag{4.4}$$

and

$$\mathbf{n} \cdot \nu(x, y)\delta(x, y)(\nabla_\rho - \alpha(x, y))\phi_n(x, y) = \begin{cases} \text{continuous (at interfaces)}, \\ 0 \text{ (at surfaces)}. \end{cases} \tag{4.5}$$

We denote $\mathbf{n} \cdot \nabla_\rho$ by $\partial/\partial n$. Since the degrees of freedom of shape functions are limited, we cannot satisfy all the boundary conditions at interfaces of elements in general.

After specifying the values of ϕ at three vertices, seven are left for each element. In order to satisfy the continuity of ϕ on three sides, we have to specify, at each node, the derivative of ϕ along two sides meeting there and take their values in common with adjacent elements: On each side, ϕ is a polynomial of third order of a parameter which changes linearly with the distance from one node, and values and derivatives on both ends completely determine ϕ. We thus need six of remaining degrees of freedom.

Since there remains only one degree of freedom, we are not able to take explicitly into account the boundary conditions on the derivatives of ϕ normal to interfaces. Instead, we use it to specify the value at the center of mass P_G.

In this case the shape functions for the element determined by P_1, P_2, and P_3 above are

$$N_1 = \xi_1 \left(3\xi_1 - 2\xi_1^2 - 7\xi_2\xi_3\right), \tag{4.6}$$

$$N_2 = \xi_2 \left(3\xi_2 - 2\xi_2^2 - 7\xi_3\xi_1\right), \tag{4.7}$$

$$N_3 = \xi_3 \left(1 + \xi_1 + \xi_2 - 2\xi_1^2 - 2\xi_2^2 - 11\xi_1\xi_2\right), \tag{4.8}$$

$$N_G = 27\xi_1\xi_2\xi_3, \tag{4.9}$$

$$N_{23} = (x_{23}^2 + y_{23}^2)^{1/2}\xi_2\xi_3(\xi_2 - \xi_1), \tag{4.10}$$

$$N_{32} = (x_{23}^2 + y_{23}^2)^{1/2}\xi_2\xi_3(\xi_3 - \xi_1), \tag{4.11}$$

$$N_{31} = (x_{31}^2 + y_{31}^2)^{1/2}\xi_3\xi_1(\xi_3 - \xi_2), \tag{4.12}$$

$$N_{13} = (x_{31}^2 + y_{31}^2)^{1/2}\xi_3\xi_1(\xi_1 - \xi_2), \tag{4.13}$$

$$N_{12} = (x_{12}^2 + y_{12}^2)^{1/2}\xi_1\xi_2(\xi_1 - \xi_3), \tag{4.14}$$

$$N_{21} = (x_{12}^2 + y_{12}^2)^{1/2}\xi_1\xi_2(\xi_2 - \xi_3), \tag{4.15}$$

where $x_{ij} = x_i - x_j$, *etc.* These functions are characterized by four values at three vertices and the center of mass together with two derivatives along two sides at each vertex;

$$N_i(P_j) = \delta_{ij},\ N_i(P_G) = \mathbf{p}_{ij} \cdot \nabla_\rho N_k(P_l) = 0, \tag{4.16}$$

$$N_G(P_G) = 1,\ N_G(P_i) = \mathbf{p}_{ij} \cdot \nabla_\rho N_k(P_l) = 0, \tag{4.17}$$

$$\mathbf{p}_{ij} \cdot \nabla_\rho N_{ji}(P_k) = \delta_{jk},\ N_{ij}(P_k) = 0,\ N_{ij}(P_G) = 0. \tag{4.18}$$

Here

$$\mathbf{p}_{ij} = (\mathbf{P}_i - \mathbf{P}_j)/\mid \mathbf{P}_i - \mathbf{P}_j \mid, \tag{4.19}$$

$\mathbf{P}_i$ is the position of the vertex P_i, and $i, j, k, l = 1, 2, 3$.

One of another possibilities may be to satisfy the continuities of ϕ and $\nu\delta\partial\phi/\partial n$ at the center of three sides in the expense of six degrees of freedom. In this case, the value of ϕ becomes discontinuous on the sides when we move from one element to another: Third order polynomial is not uniquely determined by values at three points.

It is also possible to specify two derivatives in x- and y- directions at three vertices. The shape functions are then given by

$$N_1 = \xi_1 \left(3\xi_1 - 2\xi_1^2 - 7\xi_2\xi_3\right), \tag{4.20}$$

$$N_2 = \xi_2 \left(3\xi_2 - 2\xi_2^2 - 7\xi_3\xi_1\right), \tag{4.21}$$

$$N_3 = \xi_3 \left(1 + \xi_1 + \xi_2 - 2\xi_1^2 - 2\xi_2^2 - 11\xi_1\xi_2\right), \tag{4.22}$$

$$N_G = 27\xi_1\xi_2\xi_3, \tag{4.23}$$

$$\tilde{N}_{1x} = \xi_1[x_{31}\xi_1(1-\xi_1) + (2x_1 - x_2 - x_3)\xi_2(1-\xi_2) - 2x_{12}\xi_1\xi_2], \tag{4.24}$$

$$\tilde{N}_{1y} = \xi_1[y_{31}\xi_1(1-\xi_1) + (2y_1 - y_2 - y_3)\xi_2(1-\xi_2) - 2y_{12}\xi_1\xi_2], \tag{4.25}$$

$$\tilde{N}_{2x} = \xi_2[-x_{12}\xi_2(1-\xi_2) + (2x_2 - x_1 - x_3)\xi_1(1-\xi_1) + 2x_{12}\xi_1\xi_2], \tag{4.26}$$

$$\tilde{N}_{2y} = \xi_2[-y_{12}\xi_2(1-\xi_2) + (2y_2 - y_1 - y_3)\xi_1(1-\xi_1) + 2y_{12}\xi_1\xi_2], \tag{4.27}$$

$$\tilde{N}_{3x} = \xi_3[-x_{31}\xi_1(1-\xi_1) + x_{23}\xi_2(1-\xi_2) + 2(2x_3 - x_1 - x_2)\xi_1\xi_2], \tag{4.28}$$

$$\tilde{N}_{3y} = \xi_3[-y_{31}\xi_1(1-\xi_1) + y_{23}\xi_2(1-\xi_2) + 2(2y_3 - y_1 - y_2)\xi_1\xi_2]. \tag{4.29}$$

These function are characterized by the values and derivatives at vertices and the center of mass as

$$N_i(P_j) = \delta_{ij},\ N_i(P_G) = \frac{\partial}{\partial x}N_i(P_j) = \frac{\partial}{\partial y}N_i(P_j) = 0, \tag{4.30}$$

$$N_G(P_G) = 1,\ N_G(P_i) = \frac{\partial}{\partial x}N_G(P_i) = \frac{\partial}{\partial y}N_G(P_i) = 0, \tag{4.31}$$

$$\frac{\partial}{\partial x}\tilde{N}_{ix}(P_j) = \delta_{ij},\ \tilde{N}_{ix}(P_j) = \tilde{N}_{ix}(P_G) = \frac{\partial}{\partial y}\tilde{N}_{ix}(P_j) = 0, \tag{4.32}$$

$$\frac{\partial}{\partial y}\tilde{N}_{iy}(P_j) = \delta_{ij},\ \tilde{N}_{iy}(P_j) = \tilde{N}_{iy}(P_G) = \frac{\partial}{\partial x}\tilde{N}_{iy}(P_j) = 0, \tag{4.33}$$

where $i, j = 1, 2, 3$. We may then define $N_{1x}, \ldots, N_{3y}$ as

$$N_{ix} = \frac{\tilde{N}_{ix}}{\nu\delta_i}, \tag{4.34}$$

$$N_{iy} = \frac{\tilde{N}_{iy}}{\nu\delta_i}, \tag{4.35}$$

where $\nu\delta_i$ is the value of $\nu(x,y)\delta(x,y)$ at P_i (or limiting value from inside of the element when discontinuous),

$$\nu\delta_i = \nu(P_i)\delta(P_i) \tag{4.36}$$

and impose the continuities of $\nu\delta\partial\phi/\partial x$ and $\nu\delta\partial\phi/\partial y$ at three nodes. In this case, however, the tangential component of $\nu\delta\nabla\phi$ also satisfy the same boundary conditions as the normal component instead of the correct ones and the discontinuity of ϕ appears.

Considering that the condition on ϕ is more fundamental and the simplicity of numerical procedures, we adopt the continuity of ϕ along the sides as the conditions to be satisfied by the remaining freedom in what follows.

C. Galerkin Equation

We express the solution as a superposition of the above shape functions as

$$\phi = \sum_{l=1}^{n} \left[N_1^{(l)} N_2^{(l)} N_3^{(l)} N_G^{(l)} N_{23}^{(l)} \dots N_{21}^{(l)} \right] \begin{bmatrix} \phi_1^{(l)} \\ \phi_2^{(l)} \\ \vdots \\ \phi_{21}^{(l)} \end{bmatrix}, \tag{4.37}$$

and rewrite the original equation into the weak form by taking the inner product with the function ψ which has the same form as ϕ:

$$(\psi, (\mathcal{L} - \varepsilon)\phi) = 0, \tag{4.38}$$

where

$$\psi = \sum_{l=1}^{n} \left[\psi_1^{(l)} \psi_2^{(l)} \dots \psi_{21}^{(l)} \right] \begin{bmatrix} N_1^{(l)} \\ N_2^{(l)} \\ N_3^{(l)} \\ N_G^{(l)} \\ N_{23}^{(l)} \\ \vdots \\ N_{21}^{(l)} \end{bmatrix}. \tag{4.39}$$

We thus have

$$\int_D dxdy\, \nu \sum_{l,m=1}^{n} \left[\psi_1^{(l)} \psi_2^{(l)} \dots \psi_{21}^{(l)} \right] \begin{bmatrix} N_1^{(l)} \\ N_2^{(l)} \\ \vdots \\ N_{21}^{(l)} \end{bmatrix} (\mathcal{L} - \varepsilon) \left[N_1^{(m)} N_2^{(m)} \dots N_{21}^{(m)} \right] \begin{bmatrix} \phi_1^{(m)} \\ \phi_2^{(m)} \\ \vdots \\ \phi_{21}^{(m)} \end{bmatrix}$$

$$= \sum_{l=1}^{n} \left[\psi_1^{(l)} \psi_2^{(l)} \dots \psi_{21}^{(l)} \right] \left[F_{ij}^{(l)} \right] \begin{bmatrix} \phi_1^{(l)} \\ \phi_2^{(l)} \\ \vdots \\ \phi_{21}^{(l)} \end{bmatrix} = 0. \tag{4.40}$$

Here

$$\left[F_{ij}^{(l)} \right] = \left[K_{ij}^{(l)} \right] - \varepsilon \left[M_{ij}^{(l)} \right] + \left[D_{ij}^{(l)} \right], \tag{4.41}$$

$$K_{ij}^{(l)} = \int_{(l)} dxdy\nu\delta \nabla N_i^{(l)} \cdot \nabla N_j^{(l)}, \tag{4.42}$$

$$M_{ij}^{(l)} = \int_{(l)} dxdy\nu N_i^{(l)} N_j^{(l)}, \tag{4.43}$$

and $\left[D_{ij}^{(l)} \right]$ is defined for elements on the boundary as

$$D_{ij}^{(l)} = \int_{\partial(l)} d\sigma \nu \delta N_i^{(l)} \frac{\partial}{\partial n} N_j^{(l)}. \tag{4.44}$$

Final equations are obtained by setting the coefficient of $\psi_i^{(l)}$ at each node to be zero, or by superposing

$$\left[F_{ij}^{(l)}\right] \begin{bmatrix} \phi_1^{(l)} \\ \phi_2^{(l)} \\ \vdots \\ \phi_{21y}^{(l)} \end{bmatrix} = 0 \tag{4.45}$$

so as to collect coefficients for the same node coming from neighboring elements.

D. Boundary Conditions

In our case, the boundary condition at the surface is

$$\frac{\partial}{\partial n}\phi = 0. \tag{4.46}$$

This is a typical case of the natural boundary condition. Therefore our solution is obtained from the equation for $\phi_i^{(l)}$ for all nodes with $\left[D_{ij}^{(l)}\right] = 0$.

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