

# QUANTUM MECHANICS TEXT

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## 1 Matrix Formulation of the Schrödinger Equation

Schrödinger's first formulation of the new quantum theory was as a variational principle. He proposed that the solutions  $\psi(x)$  that made a certain action functional stationary held physical significance. The action functional proposed by Schrödinger is

$$I = \int \left[ \left( \left( \mathbf{p} - \frac{q}{c} \mathbf{A} \right) \psi(x) \right)^* \cdot \left( \left( \mathbf{p} - \frac{q}{c} \mathbf{A} \right) \psi(x) \right) + V(x) \psi^*(x) \psi(x) \right] dV \quad (1)$$

He looked for functions  $\psi(x)$  for which this action integral was stationary, subject to the condition that the wavefunctions did not go to zero:  $\int \psi^*(x) \psi(x) dV = 1$ .

When the normalization condition on the wavefunctions is imposed using Lagrange multipliers, and the action integral is integrated by parts, Schrödinger's well-known second order partial differential equation results.

Another way to search for quantum solutions is to choose a set of basis functions  $f_i(x)$  and expand the unknown functions  $\psi(x)$  in terms of this basis:  $\psi(x) = \sum_j c_j f_j(x)$ . In principle the sum should extend to "infinity" (countable or uncountable, depending on the potential); in practice we will always truncate the sum at some (large) finite value and hope (or test) for convergence. The approximations to the wavefunctions  $\psi(x)$  depend *linearly* on the unknown expansion coefficients  $c_j$ . The action integral depends quadratically on the wavefunctions  $\psi(x)$  (or linearly on  $\psi$  and also on  $\psi^*(x)$ ). As a result the action integral depends quadratically (or bilinearly) on  $c_j^* c_k$ . The coefficients of these terms can be constructed by opening up the parentheses in the action integral. We find the following result

$$I \xrightarrow{\psi \rightarrow \sum_j c_j f_j(x)} \sum_{j,k} c_j^* \{ \mathcal{K} + \mathcal{M} + \mathcal{V} - \lambda \mathcal{O} \}_{j,k} c_k \quad (2)$$

The constraint condition  $\int \psi^*(x)\psi(x) dV = 1$  is enforced by the Lagrange multiplier  $\lambda$ , which will have an interpretation as an energy eigenvalue. The four matrices that appear within the brackets  $\{\}$  are the kinetic energy matrix  $\mathcal{K}$ , the potential energy matrix  $\mathcal{V}$ , the magnetic matrix  $\mathcal{M}$ , and the overlap matrix  $\mathcal{O}$ . These matrices are defined by

$$\begin{aligned}\mathcal{K}_{j,k} &= \frac{\hbar^2}{2m} \int \nabla f_j^*(x) \cdot \nabla f_k(x) dV \\ \mathcal{M}_{j,k} &= \frac{q\hbar/i}{2mc} \int \left[ -\nabla f_j^*(x) \cdot \mathbf{A} f_k(x) + f_j^*(x) \mathbf{A} \cdot \nabla f_k(x) \right] dV \\ \mathcal{V}_{j,k} &= \int f_j^*(x) \left[ V(x) + \frac{q^2}{2mc^2} \mathbf{A} \cdot \mathbf{A} \right] f_k(x) dV \\ \mathcal{O}_{j,k} &= \int f_j^*(x) f_k(x) dV\end{aligned}\tag{3}$$

If the magnetic term is absent (e.g.,  $q = 0$  or  $\mathbf{A} = \mathbf{0}$ ) and only bound states are sought, all coefficients  $c_j$  can be assumed to be real. If the magnetic term is nonzero, it is convenient to lump the diamagnetic term ( $\frac{q^2}{2mc^2} \mathbf{A} \cdot \mathbf{A}$ ) with the potential  $V(x)$ .

The quadratic form in Eq. (2) is made stationary by varying the coefficients  $c_j$ . This leads directly to the matrix eigenvalue equation:

$$\delta I = 0 \Rightarrow \sum_k \{\mathcal{K} + \mathcal{M} + \mathcal{V} - \lambda \mathcal{O}\}_{j,k} c_k = 0\tag{4}$$

It is clear from the expressions above that the devil is in the details of the set of functions  $f_j(x)$  used to approximate the wavefunctions  $\psi(x)$ .

**Remark:** If a magnetic field is present, one must first compute the vector potential that represents the field. This is done through well-known integral relations (Helmholtz theorem). If  $\mathbf{B}(\mathbf{x})$  is the magnetic field, then its vector potential  $\mathbf{A}(\mathbf{x})$  is obtained through the volume and surface integrals

$$\mathbf{A}(\mathbf{x}) = \frac{1}{4\pi} \nabla \times \int_V \frac{\mathbf{B}(\mathbf{y})}{\|\mathbf{x} - \mathbf{y}\|} dV + \frac{1}{4\pi} \int_{\partial V} \frac{\mathbf{B}(\mathbf{y})}{\|\mathbf{x} - \mathbf{y}\|} \times d\mathbf{S}\tag{5}$$

Then  $\nabla \times \mathbf{A}(\mathbf{x}) = \mathbf{B}(\mathbf{x})$ .

## 2 Gaussian Basis

### 2.1 Possible Basis Functions

One possible choice of functions is the Taylor series expansion of  $\psi(x)$  about some point in the configuration space:

$$\psi(\mathbf{x}) = \psi_{\mathbf{a}} + (\mathbf{x} - \mathbf{a})_i \psi_{\mathbf{a},i} + \frac{1}{2!} (\mathbf{x} - \mathbf{a})_i (\mathbf{x} - \mathbf{a})_j \psi_{\mathbf{a},ij} + \dots \quad (6)$$

Under this ansatz the functions  $f_*(x)$  are  $1, (\mathbf{x} - \mathbf{a})_i, (\mathbf{x} - \mathbf{a})_i (\mathbf{x} - \mathbf{a})_j, \dots$  and the unknown coefficients  $c_*$  are the Taylor series coefficients  $\psi_{\mathbf{a}}, \psi_{\mathbf{a},i}, \psi_{\mathbf{a},ij}, \dots$ . Such a choice comes endowed with too many problems.

A better choice involves expansions around many different points in the part of the configuration space of interest. In order to prevent extreme overlap of the expansions about different points, the expansion about each vertex  $\mathbf{a}$  will be highly tempered by multiplication by a function that decreases rapidly as the distance from the vertex  $\mathbf{a}$  increases. A convenient set of functions with this property consists of the gaussian-modulated Taylor series about many vertices:

$$f_*(x) = \left( \psi_{\mathbf{a}} + (\mathbf{x} - \mathbf{a})_i \psi_{\mathbf{a},i} + \frac{1}{2!} (\mathbf{x} - \mathbf{a})_i (\mathbf{x} - \mathbf{a})_j \psi_{\mathbf{a},ij} + \dots \right) \times f(\mathbf{x}; \mathbf{a}, A) \quad (7)$$

It is convenient to choose  $f(\mathbf{x}; \mathbf{a}, A)$  as a multidimensional gaussian with maximum value 1 at vertex  $\mathbf{a}$  with positive definite covariance matrix  $A$ :

$$f(\mathbf{x}; \mathbf{a}, A) = e^{-(\mathbf{x}-\mathbf{a})^t A (\mathbf{x}-\mathbf{a})} \quad (8)$$

There are as many basis functions centered around the vertex  $\mathbf{a}$  as there are terms retained in the Taylor series expansion.

### 2.2 Elementary Integrals

Before proceeding, we consider the elementary one-dimensional integrals

$$I^{(0)} = \int_{-\infty}^{+\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}} \quad I^{(2)} = \int_{-\infty}^{+\infty} x^2 e^{-\alpha x^2} dx = \frac{1}{2} \alpha^{-1} I^{(0)} \quad (9)$$

If we know the value of the wavefunction at a sufficient number of points in a region of space, we have a good approximation to it. Accordingly,

we create a tessellation of space and create an approximation to the wave function through an expression of the form  $\psi(\mathbf{x}) \simeq \sum_{\mathbf{a}} \psi_{\mathbf{a}} f(\mathbf{x}; \mathbf{a})$ , where  $\psi_{\mathbf{a}}$  is the approximate value of the wavefunction at vertex  $\mathbf{a}$  and the function  $f(\mathbf{x}; \mathbf{a})$  is highly localized around this vertex. That is, for the moment we retain only the first term in the Taylor series expansion about each vertex  $\mathbf{a}$ .

The amplitudes  $\psi_{\mathbf{a}}$  will be determined by converting Schrödinger's partial differential eigenvalue equation to a matrix eigenvalue equation.

### 2.3 Multidimensional Counterparts

Before proceeding it is useful to identify two integrals, generalizations of those in Eq. (9), that will appear often below. These are integrals over all space, so that the coordinates  $\mathbf{x}$  and vertex locations  $\mathbf{a}$  are dummy variables.

$$I^{(0)}(A) = \int .. \int f(\mathbf{x}; \mathbf{a}, A) d^n x = \frac{\pi^{n/2}}{\sqrt{\det(A)}} \quad (10)$$

$$I_{ij}^{(2)}(A) = \int .. \int (\mathbf{x} - \mathbf{a})_i (\mathbf{x} - \mathbf{a})_j f(\mathbf{x}; \mathbf{a}, A) d^n x = \frac{1}{2} (A^{-1})_{ij} I^{(0)}(A) \quad (11)$$

### 2.4 Completing the Square

Gaussians have the useful property that products of gaussians remain gaussians. We will repeatedly encounter integrals of functions multiplied by products of two gaussians. The product itself has the form

$$f(\mathbf{x}; \mathbf{a}, A) f(\mathbf{x}; \mathbf{b}, B) = f(\mathbf{x}; \mathbf{c}, C) e^{-\text{stuff}} \quad (12)$$

The parameters in this product can be computed by “completing the square”. The (negative of the) sum of the terms in the exponents of the two gaussian functions is

$$(\mathbf{x} - \mathbf{a})^t A (\mathbf{x} - \mathbf{a}) + (\mathbf{x} - \mathbf{b})^t B (\mathbf{x} - \mathbf{b}) = (\mathbf{x} - \mathbf{c})^t C (\mathbf{x} - \mathbf{c}) + \text{stuff} \quad (13)$$

By comparing terms in Eq. (13) we find:

$$\begin{aligned} C &= A + B \\ C\mathbf{c} &= A\mathbf{a} + B\mathbf{b} \\ \text{stuff} &= \mathbf{a}^t A \mathbf{a} + \mathbf{b}^t B \mathbf{b} - \mathbf{c}^t C \mathbf{c} \end{aligned} \quad (14)$$

The last term in the last line is  $(C\mathbf{c})^t(C^{-1})(C\mathbf{c})$ .

When “stuff”  $> 20$ , the integral is zero for all practical purposes, and need not even be computed. In making this simplification we will create matrices that are “sparse”. Fast matrix diagonalization techniques have been developed to handle sparse matrices.

The three integrals that we find useful are:

$$\begin{aligned} \int f(\mathbf{x}; \mathbf{a}, A)f(\mathbf{x}; \mathbf{b}, B) &= \mathcal{O}_{\mathbf{a},\mathbf{b}} = I^{(0)}(C)e^{-\text{stuff}} \\ \int (\mathbf{x} - \mathbf{r}_1)_i f(\mathbf{x}; \mathbf{a}, A)f(\mathbf{x}; \mathbf{b}, B) &= (\mathbf{c} - \mathbf{r}_1)_i \mathcal{O}_{\mathbf{a},\mathbf{b}} \\ \int (\mathbf{x} - \mathbf{r}_1)_i (\mathbf{x} - \mathbf{r}_2)_j f(\mathbf{x}; \mathbf{a}, A)f(\mathbf{x}; \mathbf{b}, B) &= \left( (\mathbf{c} - \mathbf{r}_1)_i (\mathbf{c} - \mathbf{r}_2)_j + \frac{1}{2}(C^{-1})_{ij} \right) \mathcal{O}_{\mathbf{a},\mathbf{b}} \end{aligned} \quad (15)$$

### 3 Wave Equation to Matrix Equation

In order to construct wavefunctions we must construct three matrices, or more accurately, quadratic forms, in the amplitudes  $\psi_{\mathbf{a}}$ . One quadratic form is defined by the kinetic energy term in the variational form of Schrödinger’s equation. A second is defined by the potential energy. The third quadratic form is the matrix of overlap integrals. We construct the matrix elements of the overlap form first.

#### 3.1 Overlap Matrix

The overlap quadratic form is

$$\int \sum_{\mathbf{a}} \psi_{\mathbf{a}}^* f(\mathbf{x}; \mathbf{a}, A) \sum_{\mathbf{b}} \psi_{\mathbf{b}} f(\mathbf{x}; \mathbf{b}, B) d^n x = \sum_{\mathbf{a},\mathbf{b}} \psi_{\mathbf{a}}^* \mathcal{O}_{\mathbf{a},\mathbf{b}} \psi_{\mathbf{b}} \quad (16)$$

The overlap matrix element  $\mathcal{O}_{\mathbf{a},\mathbf{b}}$  is given in the first of Eqs. (15).

#### 3.2 Potential Energy Matrix

The quadratic form describing the potential energy is obtained following the machinery developed to compute the overlap matrix in Eq. (16)

$$\int \sum_{\mathbf{a}} \psi_{\mathbf{a}}^* f(\mathbf{x}; \mathbf{a}, A) V(\mathbf{x}) \sum_{\mathbf{b}} \psi_{\mathbf{b}} f(\mathbf{x}; \mathbf{b}, B) d^n x = \sum_{\mathbf{a}, \mathbf{b}} \psi_{\mathbf{a}}^* \mathcal{V}_{\mathbf{a}, \mathbf{b}} \psi_{\mathbf{b}} \quad (17)$$

The potential energy is expanded about  $\mathbf{c}$  in a Taylor series to second order:

$$V(\mathbf{x}) \rightarrow V(\mathbf{c}) + V_i(\mathbf{c})(\mathbf{x} - \mathbf{c})_i + \frac{1}{2} V_{ij}(\mathbf{c})(\mathbf{x} - \mathbf{c})_i (\mathbf{x} - \mathbf{c})_j + \text{h.o.t.} \quad (18)$$

The integral over the constant term is proportional to the overlap matrix element:  $V(\mathbf{c}) \mathcal{O}_{\mathbf{a}, \mathbf{b}}$ . The integral over the linear term is zero “by symmetry”. This leaves only the integral over the quadratic term, which is  $\frac{1}{2} \text{tr}(V_{*,*} C^{-1}) \times \frac{1}{2} \mathcal{O}_{\mathbf{a}, \mathbf{b}}$ . The net result is

$$\mathcal{V}_{\mathbf{a}, \mathbf{b}} = \left( V(\mathbf{c}) + \frac{1}{4} \text{tr}(V_{*,*}(\mathbf{c}) C^{-1}) \right) \times \mathcal{O}_{\mathbf{a}, \mathbf{b}} \quad (19)$$

### 3.3 Kinetic Energy Matrix

The quadratic form describing the kinetic energy is obtained following the prescriptions above.

$$\frac{\hbar^2}{2m} \times \int \sum_{\mathbf{a}} \psi_{\mathbf{a}}^* \frac{\partial}{\partial x_i} f(\mathbf{x}; \mathbf{a}, A) \sum_{\mathbf{b}} \psi_{\mathbf{b}} \frac{\partial}{\partial x_i} f(\mathbf{x}; \mathbf{b}, B) d^n x = \sum_{\mathbf{a}, \mathbf{b}} \psi_{\mathbf{a}}^* \mathcal{K}_{\mathbf{a}, \mathbf{b}} \psi_{\mathbf{b}} \quad (20)$$

The derivatives are easy to take. We find

$$\mathcal{K}_{\mathbf{a}, \mathbf{b}} = \frac{\hbar^2}{2m} \times \int 2A_{ir}(\mathbf{x} - \mathbf{a})_r \times 2B_{is}(\mathbf{x} - \mathbf{b})_s \times f(\mathbf{x}; \mathbf{a}, A) f(\mathbf{x}; \mathbf{b}, B) d^n x \quad (21)$$

The linear terms are expanded about  $\mathbf{c}$ :  $\mathbf{x} - \mathbf{b} = (\mathbf{x} - \mathbf{c}) + (\mathbf{c} - \mathbf{b})$  and the integrals are carried out using the third of Eqs. (15):

$$\mathcal{K}_{\mathbf{a}, \mathbf{b}} = \frac{\hbar^2}{2m} \times \left( 4(\mathbf{c} - \mathbf{a})_r (AB)_{rs} (\mathbf{c} - \mathbf{b})_s + 2\text{tr}(ABC^{-1}) \right) \times \mathcal{O}_{\mathbf{a}, \mathbf{b}} \quad (22)$$

### 3.4 Magnetic Terms

In order to account for the effects of magnetic fields it is necessary to compute integrals of the form

$$\frac{1}{2m} \int \left( \frac{\hbar}{i} \nabla - \frac{q}{c} \mathbf{A} \right) \psi^* \cdot \left( \frac{\hbar}{i} \nabla - \frac{q}{c} \mathbf{A} \right) \psi dV \quad (23)$$

Of the four terms in this product, the first  $(\nabla\psi^*\nabla\psi)$  is the kinetic energy term. It has been treated above and the matrix expression for the kinetic energy is given in Eq. (22). The term lacking the gradient is  $\psi^* \frac{q^2}{2mc^2} \mathbf{A} \cdot \mathbf{A} \psi$ . This diamagnetic term can be treated as if it were a contribution to the potential energy. It's matrix has the form given in Eq.(19). The two cross-product terms are

$$- \frac{1}{2m} \int \left( \frac{\hbar}{i} \nabla \psi \right)^* \cdot \frac{q}{c} \mathbf{A} \psi + \frac{q}{c} \mathbf{A} \psi^* \cdot \left( \frac{\hbar}{i} \nabla \psi \right) dV \quad (24)$$

The product of the two gaussians is  $f(\mathbf{x}; \mathbf{c}, C)e^{-\text{stuff}}$  as usual. The vector potential is expanded around  $\mathbf{c}$  to first order:  $A_i(\mathbf{x}) \simeq A_i(\mathbf{c}) + A_{i,r}(\mathbf{c})(\mathbf{x} - \mathbf{c})_r + \dots$ . When these expressions are placed into the integral and appropriately carried out, we find

$$\mathcal{M}_{\mathbf{a},\mathbf{b}} = \frac{q\hbar/i}{2mc} \left[ 2\mathbf{A}_r(\mathbf{c}) (A_{rs}(\mathbf{c} - \mathbf{a})_s - B_{rs}(\mathbf{c} - \mathbf{b})_s) + \mathbf{A}_{r;s} (A - B)_{rt} C_{ts}^{-1} \right] \times \mathcal{O}_{\mathbf{a},\mathbf{b}} \quad (25)$$

### 3.5 Eigenvalues and Eigenfunctions

Once the matrix elements of the kinetic energy operator, the potential energy operator and the magnetic operator have been constructed, the variational problem to be solved is

$$\delta \left( \sum_{\mathbf{a},\mathbf{b}} \psi_{\mathbf{a}}^* (\mathcal{K}_{\mathbf{a},\mathbf{b}} + \mathcal{V}_{\mathbf{a},\mathbf{b}} + \mathcal{M}_{\mathbf{a},\mathbf{b}}) \psi_{\mathbf{b}} \right) = 0 \quad \sum_{\mathbf{a},\mathbf{b}} \psi_{\mathbf{a}}^* \mathcal{O}_{\mathbf{a},\mathbf{b}} \psi_{\mathbf{b}} = 1 \quad (26)$$

This leads, in the usual way (via Lagrange multipliers) to a standard eigenvalue equation. The energy eigenvalues and eigenvectors are determined by solving the generalized eigenvalue equation

$$\sum_{\mathbf{b}} (\mathcal{K}_{\mathbf{a},\mathbf{b}} + \mathcal{V}_{\mathbf{a},\mathbf{b}} + \mathcal{M}_{\mathbf{a},\mathbf{b}} - \lambda \mathcal{O}_{\mathbf{a},\mathbf{b}}) \psi_{\mathbf{b}} = 0 \quad (27)$$

The eigenvalues  $\lambda_1, \lambda_2, \dots$  are the energy eigenvalues  $E_\alpha, \alpha = 1, 2, \dots$  and the amplitudes  $\psi_{\mathbf{b}}(\alpha)$  are the coefficients of the basis functions  $f(\mathbf{x}; \mathbf{b}, B)$  of the  $\alpha$ th eigenvector at vertex  $\mathbf{b}$ . The eigenvectors satisfy the orthogonality relations

$$\sum_{\mathbf{a}, \mathbf{b}} \psi_{\mathbf{a}}^*(\alpha) \mathcal{O}_{\mathbf{a}, \mathbf{b}} \psi_{\mathbf{b}}(\beta) = \delta(\alpha, \beta) \quad (28)$$

The wavefunction for the energy  $E_\alpha$  is constructed from the eigenvectors  $\psi_{\mathbf{b}}(\alpha)$  by constructing the proper superposition of basis vectors:

$$\psi_\alpha(\mathbf{x}) = \sum_{\mathbf{b}} \psi_{\mathbf{b}}(\alpha) f(\mathbf{x}; \mathbf{b}, B) \quad (29)$$

These wavefunctions can be evaluated for any value of the position coordinate  $\mathbf{x}$  in the domain tessellated. Ordinarily the values of the wavefunction are determined at the vertices, so that

$$\psi_\alpha(\mathbf{a}) = \sum_{\mathbf{b}} \psi_{\mathbf{b}}(\alpha) f(\mathbf{a}; \mathbf{b}, B) = \sum_{\mathbf{b}} \psi_{\mathbf{b}}(\alpha) e^{-(\mathbf{a}-\mathbf{b}^t)B(\mathbf{a}-\mathbf{b})} \quad (30)$$

The values of  $e^{-(\mathbf{a}-\mathbf{b}^t)B(\mathbf{a}-\mathbf{b})}$  can be considered as the elements of a matrix  $M_{\mathbf{a},\mathbf{b}}(B)$  that is not symmetric, so that the value of the eigenfunctions can finally be expressed as a matrix product:

$$\psi_\alpha(\mathbf{a}) = \sum_{\mathbf{b}} M_{\mathbf{a},\mathbf{b}}(B) \psi_{\mathbf{b}}(\alpha) \quad (31)$$

Matrix elements of  $M_{\mathbf{a},\mathbf{b}}(B)$  that are sufficiently small can be zeroed out to save computational complexity.

## 4 Degrees of Freedom

At this point it would be useful to extend the model of the wavefunction by introducing additional degrees of freedom at each node. The wave functions localized around each of the vertices is expanded and the expansion coefficients are used as additional degrees of freedom. The wavefunction is approximated as



$$\psi(\mathbf{x}) = \sum_{\mathbf{a}} \left( \psi_{\mathbf{a}} + \sum_i \psi_{\mathbf{a},i}(\mathbf{x} - \mathbf{a})_i + \frac{1}{2!} \psi_{\mathbf{a},ij}(\mathbf{x} - \mathbf{a})_i(\mathbf{x} - \mathbf{a})_j + \dots \right) \times f(\mathbf{x}; \mathbf{a}, A) \quad (32)$$

In the following we will use just the leading (constant  $\psi_{\mathbf{a}}$  and linear  $\psi_{\mathbf{a},i}$ ) terms from each localized wavefunction. The constant terms at each vertex  $\mathbf{a}$  are labelled with an index  $\mu$ , where  $\mu = (0, 1, 2, 3)$  and  $\mu = 0$  refers to the value of the wavefunction and the indices  $\mu = i$  to the components of its gradient:  $\psi_{\mu}(\mathbf{a}) \rightarrow (\psi(\mathbf{a}), \partial_1 \psi(\mathbf{a}), \psi_2(\mathbf{a}), \psi_3(\mathbf{a}))$ .

This ansatz of Eq. (32) must be put through the machines outlined above. We keep terms only up to second-order smallness  $\simeq |\mathbf{b} - \mathbf{a}|^2$  in these calculations. The results are as follows:

$$\mathcal{O}_{\mathbf{a}\mu, \mathbf{b}\nu} = \left[ \frac{1}{(\mathbf{c} - \mathbf{a})_i} \middle| \frac{(\mathbf{c} - \mathbf{b})_j}{(\mathbf{c} - \mathbf{a})_i(\mathbf{c} - \mathbf{b})_j + \frac{1}{2}C_{ij}^{-1}} \right] \times \mathcal{O}_{\mathbf{a}, \mathbf{b}} \quad (33)$$

$$\begin{aligned} \mathcal{V}_{\mathbf{a}\mu, \mathbf{b}\nu} &= V(\mathbf{c}) \times \mathcal{O}_{\mathbf{a}\mu, \mathbf{b}\nu} + \frac{1}{2} \left[ \begin{array}{cc} 0 & V_k(\mathbf{c})C_{kj}^{-1} \\ C_{ik}^{-1}V_k(\mathbf{c}) & (\mathbf{c} - \mathbf{a})_i V_k(\mathbf{c})C_{kj}^{-1} + C_{ik}^{-1}V_k(\mathbf{c})(\mathbf{c} - \mathbf{b})_j \end{array} \right] \times \mathcal{O}_{\mathbf{a}, \mathbf{b}} \\ &+ \frac{1}{4} \text{tr} (V_{**}(\mathbf{c})C^{-1}) \times \left[ \begin{array}{c} 1 \\ (\mathbf{c} - \mathbf{a})_i \end{array} \right] \left[ \begin{array}{cc} 1 & (\mathbf{c} - \mathbf{b})_j \end{array} \right] \times \mathcal{O}_{\mathbf{a}, \mathbf{b}} \quad (34) \end{aligned}$$

$$\mathcal{K}_{\mathbf{a}\mu, \mathbf{b}\nu} = \frac{\hbar^2}{2m} \left[ \begin{array}{c|c} \text{tr} A (4(\mathbf{c} - \mathbf{a})(\mathbf{c} - \mathbf{b}) + 2C^{-1}) B & -2(\mathbf{c} - \mathbf{a})_r A_{rj} \\ \hline -2B_{ir}(\mathbf{c} - \mathbf{b})_r & \begin{array}{c} \delta_{ij} \\ -(2(\mathbf{c} - \mathbf{a})(\mathbf{c} - \mathbf{a}) + C^{-1})_{ir} A_{rj} \\ -B_{ir} (2(\mathbf{c} - \mathbf{b})(\mathbf{c} - \mathbf{b}) + C^{-1})_{rj} \end{array} \end{array} \right] \times \mathcal{O}_{\mathbf{a}, \mathbf{b}} \quad (35)$$

$$\mathcal{M}_{\mathbf{a}\mu, \mathbf{b}\nu} = \frac{q\hbar/i}{2mc} \times \mathcal{O}_{\mathbf{a}, \mathbf{b}} \times$$

$$\left[ \begin{array}{c|c}
\begin{array}{l}
2\mathbf{A}_r(\mathbf{c}) (A_{rs}(\mathbf{c} - \mathbf{a})_s - B_{rs}(\mathbf{c} - \mathbf{b})_s) \\
+ \mathbf{A}_{r;s} (A - B)_{rt} C_{ts}^{-1}
\end{array} & \begin{array}{l}
\mathbf{A}_j(\mathbf{c}) \\
+ 2\mathbf{A}_r(\mathbf{c}) A_{rs} \left( (\mathbf{c} - \mathbf{a})(\mathbf{c} - \mathbf{b}) + \frac{1}{2}C^{-1} \right)_{sj} \\
- 2\mathbf{A}_r(\mathbf{c}) B_{rs} \left( (\mathbf{c} - \mathbf{b})(\mathbf{c} - \mathbf{b}) + \frac{1}{2}C^{-1} \right)_{sj}
\end{array} \\
\hline
\begin{array}{l}
- \mathbf{A}_i(\mathbf{c}) \\
- 2 \left( (\mathbf{c} - \mathbf{a})(\mathbf{c} - \mathbf{b}) + \frac{1}{2}C^{-1} \right)_{ir} B_{rs} \mathbf{A}_s(\mathbf{c}) \\
+ 2 \left( (\mathbf{c} - \mathbf{a})(\mathbf{c} - \mathbf{a}) + \frac{1}{2}C^{-1} \right)_{ir} A_{rs} \mathbf{A}_s(\mathbf{c})
\end{array} & \begin{array}{l}
(\mathbf{c} - \mathbf{a})_i \mathbf{A}_j(\mathbf{c}) - \mathbf{A}_i(\mathbf{c})(\mathbf{c} - \mathbf{a})_j \\
+ \frac{1}{2}C_{ir}^{-1} \mathbf{A}_{j;r}(\mathbf{c}) - \frac{1}{2} \mathbf{A}_{i;r}(\mathbf{c}) C_{jr}^{-1}
\end{array}
\end{array} \right] \quad (36)$$

## 5 Tessellation

The choice of vertices  $\mathbf{a}$  and covariance matrices  $A_{\mathbf{a}}$  should be adjusted to the potential. If the potential is smooth (i.e., harmonic  $\frac{1}{2}kx^2$ ) then a regular lattice with spherically symmetric covariance matrices ( $A \rightarrow \lambda I_n$ ) at each vertex is suitable. Acceptable eigenstates are those for which the amplitudes  $\psi_{\mathbf{a}} \rightarrow 0$  suitably fast as the boundary is approached.

If the potential is confining or the domain on which the wavefunction is supported has edges, corners, holes, ... then appropriate adjustments should be made. For example, a number of vertices should creep up to an edge, and at those vertices nearest the edge the covariance matrices should be elongated, with the long axes parallel to the edge and the short axes perpendicular. In this way it is possible to model multiply connected regions of space rather simply.