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SEMICLASSICAL ASYMPTOTICS OF EIGENVALUES FOR THE DIRAC OPERATOR WITH MAGNETIC AND ELECTRIC POTENTIALS

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Abstract: We consider the Dirac operator with magnetic and electric potentials. Our final aim is to get the asymptotic behavior of the eigenvalues in the semiclassical sense. In the particular case of single well, we get a sufficient condition for the eigenvalue to be non-degenerate and then we can give the asymptotic expansion of the eigenvalue. We also give an example which seems to be new.

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1. Introduction

In this paper, we consider the Dirac operator depending on a small parameter $h > 0$ with the electric potential $V(x)$ and the magnetic potential $a(x) = (a_1(x), a_2(x), a_3(x))$:

$$P_V^h(a) = \alpha \cdot D^h(a) + \alpha_4 + V(x)I_4, \tag{1.1}$$

on $\mathcal{H} = L^2(\mathbf{R}^3; \mathbf{C}^4)$, where $D^h(a) = (D_1^h(a), D_2^h(a), D_3^h(a))$, $D_j^h(a) = -ih\partial_j - a_j(x)$, $\partial_j = \partial/\partial x_j$, $i = \sqrt{-1}$, $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ and $\alpha \cdot D^h(a) = \sum_{j=1}^3 \alpha_j D_j^h(a)$. Here α_j $(j = 1, 2, 3, 4)$ are 4×4 Hermitian matrices on $\mathbf{C}^4$ of the forms

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$$\alpha_j = \begin{bmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{bmatrix} \quad (j=1,2,3), \quad \alpha_4 = \begin{bmatrix} I_2 & 0 \\ 0 & -I_2 \end{bmatrix},$$

where I_4 and I_2 are the identity matrices on $\mathbf{C}^4$ and $\mathbf{C}^2$, respectively and σ_j $(j=1,2,3)$ are so-called the Pauli matrices:

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

It is easily seen that the following relations hold:

$$\begin{aligned} &\sigma_1\sigma_2 = -\sigma_2\sigma_1 = i\sigma_3, \quad \sigma_2\sigma_3 = -\sigma_3\sigma_2 = i\sigma_1, \\ &\sigma_3\sigma_1 = -\sigma_1\sigma_3 = i\sigma_2, \end{aligned} \tag{1.2}$$

and hence,

$$\alpha_j\alpha_k + \alpha_k\alpha_j = 2\delta_{kj}I_4 \quad \text{for } j,k = 1,2,3,4\,, \tag{1.3}$$

where δ_{kj} is the Kronecker delta.

If we assume that the electric potential $V(x)$ is a real valued C^∞ function on $\mathbf{R}^3$ and that there exist $E \in \mathbf{R}, \epsilon > 0, R > 0$ such that $|V(x) - E| \leq 1 - \epsilon$ for $|x| \geq R$, it is well-known that the spectrum $\sigma(P_V^h(a))$ of $P_V^h(a)$ in a neighborhood of E is contained in the discrete spectrum $\sigma_{\text{disc}}(P_V^h(a))$. We call the connected components of the set $\{x \in \mathbf{R}^3; |V(x) - E| \geq 1\}$ the wells of energy E of $P_V^h(a)$.

The purpose of this paper is to study the semiclassical asymptotics of the eigenvalues near E in the case of multiple wells.

Wang [13] considered the similar problem for the Dirac operator without magnetic potential and Mohamed and Parisse [12] and obtained some results for the operator with small magnetic potential, i.e., for $P_V^h(ha)$. In both cases, we can see that the first term in the semiclassical approximation of the operator becomes a harmonic oscillator without the magnetic potential. In our case, however, we have to consider a harmonic oscillator in the uniform magnetic field as the first term.

For the Schrödinger operator, there are many articles in this direction. For example, see Abe et al [1], Aramaki [2], [3], Helffer and Mohamed [5], Helffer and Sjöstrand [7], Mohamed [11] and Matsumoto [9].

The plan of this paper is as follows. In Section 2, we state the hypotheses and preliminary remarks which are more or less known facts. In Section 3, we study the case, where the set of wells consists of a finitely discrete set. We also give an rough estimate of eigenvalues. In Section 4, we give the main theorem on the complete expansion of eigenvalues near $E = 0$ by powers of the parameter

$h > 0$. Moreover, in the case of single well, we estimate the difference of the first and the second eigenvalues. In Section 5, we give a typical example which seems to be new in the case of single well. Finally, in appendix, we calculate the concrete values of the eigenvalues.

2. Hypotheses and Preliminaries

In this section, we shall give the hypotheses and preliminary remarks. We consider the Dirac operator on $\mathcal{H} = L^2(\mathbf{R}^3; \mathbf{C}^4)$ of type (1.1):

$$P_V^h(a) = \alpha \cdot D^h(a) + \alpha_4 + V(x)I_4.$$

Throughout this paper, we suppose that the magnetic potential and electric potential are smooth:

$$a(x) = (a_1(x), a_2(x), a_3(x)) \in C^\infty(\mathbf{R}^3; \mathbf{R}^3) \text{ and } V \in C^\infty(\mathbf{R}^3; \mathbf{R}). \tag{S.1}$$

By the smoothness of $a(x)$, it follows that $P_0^h(a)$ is essentially self-adjoint on $\mathcal{H}$ starting from $C_0^\infty(\mathbf{R}^3; \mathbf{C}^4)$. We denote its unique self-adjoint extension by the same notation. If we identify the magnetic potential $a(x)$ with 1-form $\sigma_a = \sum_{j=1}^3 a_j(x)dx_j$, the magnetic field B is defined as the differential of σ_a: $B = d\sigma_a$ which can be identified with the skew-symmetric matrix $B(x) = (B_{kj}(x))_{k,j=1,2,3}$, where $B_{kj}(x) = \partial_k a_j(x) - \partial_j a_k(x)$ as usual.

It is well-known that the spectrum $\sigma(P_0^h(a))$ satisfies

$$\sigma(P_0^h(a)) \cap (-1, 1) = \emptyset\,, \tag{2.1}$$

and the domain $D(P_0^h(a))$ is equal to the subspace $\{u \in \mathcal{H}; \alpha \cdot D^h(a)u \in \mathcal{H}\}$. For these facts, see Helffer, Nourrigat and Wang [6].

Next, for brevity of the arguments, we assume that the electric potential satisfies:

$$V(x) \to 0 \quad \text{as } |x| \to \infty. \tag{V.1}$$

Then it follows from the Kato Theorem that $P_V^h(a)$ is also an essentially self-adjoint operator on $\mathcal{H}$ starting from $C_0^\infty(\mathbf{R}^3; \mathbf{C}^4)$ whose self-adjoint extension is written by the same notation in this paper. We also find that $D(P_V^h(a)) = D(P_0^h(a))$ and $\sigma_{\text{ess}}(P_V^h(a)) = \sigma_{\text{ess}}(P_0^h(a))$ (cf. [12]). Combined these facts with (2.1), we have

$$\sigma(P_V^h(a)) \cap (-1, 1) \subset \sigma_{\text{disc}}(P_V^h(a)). \tag{2.2}$$

Here and from now on, for any self-adjoint operator A, $\sigma_{\text{ess}}(A)$ and $\sigma_{\text{disc}}(A)$ denote the essential spectrum and the discrete spectrum of A, respectively.

Now we introduce the notion of wells. It is easily seen that the symbol of $P^h_V(a)$:

$$p(x,\xi) = \alpha\cdot(\xi - a(x)) + \alpha_4 + V(x)I_4$$

has two double eigenvalues $\lambda_\pm(x,\xi) = \pm\sqrt{1+|\xi-a(x)|^2} + V(x)$. Then we can see that the projection onto $\mathbf{R}^3_x$ of the set

$$\{(x,\xi)\in \mathbf{R}^3_x\times\mathbf{R}^3_\xi; \lambda_+(x,\xi) = 0 \ \text{ or } \ \lambda_-(x,\xi) = 0\}\,,$$

is equal to $U = \{x\in\mathbf{R}^3; V(x)^2 \ge 1\}$. We call the compact, connected components $U_p \quad (p = 1, 2, \ldots, N)$ of U the wells of $P^h_V(a)$. For the brevity of the notations, we write $U_p = U^+_p$ if U_p is defined by $V(x) \ge 1$ and $U_p = U^-_p$ if U_p is defined by $V(x) \le -1$.

The following proposition plays an important role in our arguments.

Proposition 2.1. *Let $\phi(x)$ be a real valued, bounded and uniformly Lipschitz function on $\mathbf{R}^3$. Then we have*

$$\begin{aligned}&\|D^h(a)(e^{\phi/h}u)\|^2 + \int e^{2\phi/h}[1-|\nabla\phi|^2 - V^2]|u|^2dx\\ &\quad = \mathrm{Re}(e^{2\phi/h}P^h_V(a)u, P^h_{-V}(a)u) - 2\mathrm{Im}(e^{2\phi/h}P^h_V(a)u, (\alpha\cdot\nabla\phi)u)\,,\end{aligned}$$

for $u\in D(P^h_0(a))$. Here $(\cdot)$ and $\|\cdot\|$ denote the inner product and the norm in $\mathcal{H}$, respectively and $|u|$ the norm of u in $\mathbf{C}^4$.

In particular, if $F_\pm \in L^\infty(\mathbf{R}^3)$ satisfy that $F_\pm \ge 0, F_+ + F_- > 0$ and $F^2_+ - F^2_- = 1 - |\nabla\phi|^2 - V^2$, we have

$$\begin{aligned}&\|D^h(a)(e^{\phi/h}u)\|^2 + \frac{1}{2}\|F_+e^{\phi/h}u\|^2\\ &\quad \le \left\|\frac{1}{F_+ + F_-}e^{\phi/h}P^h_{-V}(a)P^h_V(a)u\right\|^2 + \frac{3}{2}\|F_-e^{\phi/h}u\|^2\,,\end{aligned}$$

for $u\in C^\infty_0(\mathbf{R}^3;\mathbf{C}^4)$.

For the proof, see [13; Proposition 2.1] and [7].

We shall consider the semiclassical asymptotics of eigenvalues of $P^h_V(a)$ in an interval $I(h) = [-a_1(h), a_2(h)]$, where $a_j(h)\downarrow 0$ as $h\downarrow 0$. For such purpose, it is adequate for us to use the notion of the Agmon distance $d(x,y)$ associated with $[1-V(x)^2]_+dx^2$, where $[a]_+ = \max\{a, 0\}$ for any real a. For the various properties of the Agmon distance, see Helffer [4].

Choose $\eta > 0$ small enough so that $\widetilde{\Omega}_p(\eta) := \{x\in\mathbf{R}^3; d(x,U_p) < \eta\}$ are mutually disjoint. Moreover, choose open set $\Omega_p = \Omega_p(\eta)$ with smooth boundaries such that $U_p\subset\Omega_p(\eta)\subset\widetilde{\Omega}_p(\eta)$, respectively.

Let $\Omega \subset \mathbf{R}^3$ be a bounded, connected open set such that the boundary $\partial\Omega$ is smooth and Ω situates in one side of $\partial\Omega$. In the later, we simply say such open set regular. Then $P_0^h(a)$ has the Dirichlet realization $P_0^{h,\Omega}(a)$ on $L^2(\Omega;\mathbf{C}^4)$ which is starting from $C_0^\infty(\Omega;\mathbf{C}^2) \otimes C^\infty(\Omega;\mathbf{C}^2)$. It follows from Hörmander [8] that

$$D(P_0^{h,\Omega}(a)) = H_0^1(\Omega;\mathbf{C}^2) \otimes H^1(\Omega;\mathbf{C}^2)\,,$$

where H_0^1 and H^1 denote the standard Sobolev spaces. Similarly as preceding arguments, we can also define the Dirichlet realization $P_V^{h,\Omega}(a)$ of $P_V^h(a)$ with the domain $D(P_V^{h,\Omega}(a)) = D(P_0^{h,\Omega}(a))$.

Now, define an anti-linear operator

$$\begin{aligned} J : L^2(\Omega;\mathbf{C}^2) \otimes L^2(\Omega;\mathbf{C}^2) &\to L^2(\Omega;\mathbf{C}^2) \otimes L^2(\Omega;\mathbf{C}^2)\,, \\ u = (u_+, u_-) &\mapsto J(u) = (\sigma_2\overline{u_+}, \sigma_2\overline{u_-}). \end{aligned}$$

Then it is easily seen that $J^2 = -I$ and that $P_V^h(0)$ commutes with J.

Remark 2.2. If $E(h)$ is an eigenvalue of $P_V^{h,\Omega}(0)$ or $P_V^h(0)$ and $\mathcal{H}_{E(h)}$ is the associated eigenspace, then we see that $J\mathcal{H}_{E(h)} = \mathcal{H}_{E(h)}$ and thus $\dim \mathcal{H}_{E(h)} = 2k$ (even). Thus we can choose a basis $\{u_1, \ldots, u_{2k}\}$ of $\mathcal{H}_{E(h)}$ such that $Ju_j = u_{j+k}$ for $j = 1, 2, \ldots, k$. Moreover, in the case of non-zero magnetic field, we merely have $P_V^h(a)J = JP_V^h(-a)$.

We return to our case. We write the Dirichlet realization of $P_V^h(a)$ in Ω_p by $P_V^{h,\Omega_p}(a)$. Note that Proposition 2.1 also holds for $P_V^{h,\Omega_p}(a)$. Now, we get the following properties on exponential decay of eigenfunctions.

Lemma 2.3. *Let $I(h) = [-a_1(h), a_2(h)] \subset (-1,1)$ as above and let*

$$\begin{aligned} \sigma(P_V^h(a)) \cap I(h) &= \{\lambda_1(h), \lambda_2(h), \ldots, \lambda_M(h)\}, \\ \sigma(P_V^{h,\Omega_p}(a)) \cap I(h) &= \{\mu_{p,1}(h), \mu_{p,2}(h), \ldots, \mu_{p,m_p}(h)\}, \end{aligned}$$

for $p = 1, 2, \ldots, N$ according to their multiplicities and let $u_k, v_{p,l}$ be the associated normalized eigenfunctions corresponding to the eigenvalues $\lambda_k(h), \mu_{p,l}(h)$, respectively. Then for any $\epsilon > 0$, there exists a constant $C_\epsilon > 0$ such that for every $k = 1, 2, \ldots, M$ and $p = 1, 2, \ldots, N, l = 1, 2, \ldots, m_p$,

$$\begin{aligned} \|D^h(a)(e^{(1-\epsilon)d/h}u_k)\|^2 &+ \|e^{(1-\epsilon)d/h}u_k\|^2 \le C_\epsilon e^{2\epsilon/h}\,, \\ \|D^h(a)(e^{(1-\epsilon)d_p/h}v_{p,l})\|^2 &+ \|e^{(1-\epsilon)d_p/h}v_{p,l}\|^2 \le C_\epsilon e^{2\epsilon/h}\,, \end{aligned}$$

where $d(x) = d(x, U)$ and $d_p(x) = d(x, U_p)$.

For the proof, see [7] and [13].

Here, we want to reduce the problem for $P_V^h(a)$ to that for the direct sum of the Dirichlet realizations $P_V^{h,\Omega_p}(a)$. In order to do so, let E, F be closed subspaces of a general Hilbert space H. If we denote the orthogonal projections onto E, F by Π_E, Π_F, we can define non-symmetric distance from E to F by $\overrightarrow{d}(E,F) = \|(I - \Pi_F)\Pi_E\|$.

Then the following proposition was proved in [7] or [4].

Proposition 2.4. *Let A be a self-adjoint operator on H and $I \subset \mathbf{R}$ a compact interval. Assume that $f_1, \dots, f_N \in H$ are linearly independent and that there exist $\mu_1, \dots, \mu_N \in I$ such that*

$$Af_j = \mu_j f_j + r_j, \quad \|r_j\| \le \epsilon \quad \text{for all } j = 1, 2, \dots, N.$$

We put $E = [f_1, \dots, f_N]$ which denotes the subspace spanned by $f_1, \dots, f_N$ and $F = E_A(\sigma(A) \cap I)H$, where $E_A(\cdot)$ is the spectral measure associated to A. Moreover, we assume that there exists $a > 0$ such that

$$\sigma(A) \cap ((I + B(0, 2a)) \setminus I) = \emptyset\,,$$

where $B(0, 2a) = (-2a, 2a)$. Then we have

$$\overrightarrow{d}(E,F) \le \frac{N^{1/2}\epsilon}{a\,(\lambda_{\min})^{1/2}}\,,$$

where $\lambda_{\min}$ is the smallest eigenvalue of the $N \times N$ matrix $((f_j, f_k))$.

In order to apply the above proposition to our case, we firstly state the following result.

Proposition 2.5. *Under the hypotheses $(S.1)$ and $(V.1)$, for any $c \in (0, 1)$, there exist constants $N_0 > 0, h_0 > 0$ and $C > 0$ such that*

$$N((-c, c); P_V^h(a)) \le Ch^{-N_0} \quad \text{for } h \in (0, h_0]\,,$$

where $N((-c, c); P_V^h(a))$ denotes the number of eigenvalues of $P_V^h(a)$ in $(-c, c)$ according to multiplicities.

Proof. At first we define a quadratic form

$$q_V^h(a)(u) = (P_V^h(a)u, P_V^h(a)u \quad \text{for } u \in d(q_V^h(a)) = D(P_V^h(a)).$$

Thanks to the hypothesis (V.1), we can choose $\epsilon_0 > 0$ so that $0 < c < 1 - \epsilon_0$ and choose $C_1 > 0$ such that $|V(x)| \le \epsilon_0$ for $|x| \ge C_1$. Moreover, we can choose a covering $\{O_i\}_{i=0,1}$ of $\mathbf{R}^3$ and a partition of unity $\{\phi_i\}_{i=0,1} \subset C^\infty(\mathbf{R}^3)$ such that $\overline{O_0}$ is a compact set and $O_1 \subset \{x \in \mathbf{R}^3; |x| \geq C_1\}$, $\sum_{i=0}^1 \phi_i^2 = 1$ and $|\nabla\phi_i| \leq C_2$ for some constant $C_2 > 0$. Then an elementary calculation leads to

$$q_V^h(a)(u) = \sum_{i=0}^{1} q_V^h(a)(\phi_i u) - h^2 \sum_{i=0}^{1} \|\alpha \cdot (\nabla\phi_i)u\|^2. \tag{2.3}$$

If we put $Q_V^h(a) = P_V^h(a)^2$, it follows from the Glazman Lemma that

$$\begin{aligned} N(c^2; Q_V^h(a)) &:= N((-\infty, c^2); Q_V^h(a)) \\ &\leq \sup\{\dim F; F \subset d(q_V^h(a)),\ q_V^h(a)(u) \leq c^2\|u\|^2 \\ &\qquad \text{for all } u \in F\}. \end{aligned}$$

Since $C_0^\infty(\mathbf{R}^3; \mathbf{C}^4)$ is dense in $d(q_V^h(a))$ with respect to the graph norm, we can replace $d(q_V^h(a))$ with $C_0^\infty(\mathbf{R}^3; \mathbf{C}^4)$ in the above formula. From now on, we denote various constants independent of $h \in (0, h_0]$ by C_j $(j = 1, 2, \ldots)$. It follows from (2.3) that if $u \in F$,

$$\sum_{i=0}^{1} q_V^h(\phi_i u) \leq q_V^h(a)(u) + C_3 h^2\|u\|^2 \leq \sum_{i=0}^{1}(c^2 + C_3h^2)\|\phi_i u\|^2.$$

Accordingly we have

$$N(c^2; Q_V^h(a)) \leq \sum_{i=0}^{1} N(c^2 + C_3h^2; Q_V^{h,O_i}(a)),$$

where $Q_V^{h,O_i}(a)$ is the Dirichlet realization of $Q_V^h(a)$ in O_i. Using the relation (1.3), we have

$$\begin{aligned} q_V^h(a)(u) &= (\alpha \cdot D^h(a)u, \alpha \cdot D^h(a)u) + (\alpha \cdot D^h(a)u, Vu) \\ &\quad + (Vu, \alpha \cdot D^h(a)u) + ((1 + 2\alpha_4 V + V^2)u, u). \end{aligned}$$

By the Schwarz inequality, we see

$$q_V^h(a)(u) \geq ((1 + 2\alpha_4 V)u, u). \tag{2.4}$$

Since $|V(x)| \leq \epsilon_0$ in O_1, we see that $q_V^{h,O_1}(a)(u) \geq (1 - 2\epsilon_0)\|u\|^2$ for $u \in C_0^\infty(O_1; \mathbf{C}^4)$ because of (2.4), and therefore, $\sigma(Q_V^{h,O_i}(a)) \subset [1 - 2\epsilon_0, \infty)$. Since $c^2 + C_3h^2 < 1 - 2\epsilon_0$ for small $h > 0$, we obtain $N(c^2 + C_3h^2; Q_V^{h,O_1}) = 0$. Thus we get an inequality

$$N(c^2; Q_V^h(a)) \leq N(c^2 + C_3h^2; Q_V^{h,O_0}(a)).$$

As V is a bounded function, it is easily seen that

$$\begin{aligned} q_V^h(a)(u) &\geq \frac{1}{2}\|\alpha \cdot D^h(a)u\|^2 - C_4\|u\|^2 \\ &\geq \frac{1}{2}\|D^h(a)u\|^2 - C_4\|u\|^2 - C_5h\|u\|^2 , \end{aligned}$$

for $u \in C_0^\infty(O_0; \mathbf{C}^4)$. Since $a(x)$ is bounded in O_1, for any $\epsilon > 0$ there exists $C_\epsilon > 0$ such that

$$\begin{aligned} (D^h(a)u, D^h(a)u) &\geq \|D^h(0)u\|^2 - \{|D^h(0)u, au)| \\ &\quad +|(au, D^h(0))| + |(au, au)|\} \\ &\geq \|D^h(0)u\|^2 - \epsilon\|D^h(0)u\|^2 - C_\epsilon\|u\|^2 \\ &\geq (1-\epsilon)\|D^h(0)u\|^2 - C_\epsilon\|u\|^2. \end{aligned}$$

Here if we take $\epsilon = 1/2$, we have

$$q_V^h(a)(u) + C_6\|u\|^2 \geq \frac{1}{4}q_0^h(0)(u) \quad \text{for } u \in C_0^\infty(O_0; \mathbf{C}^4).$$

As a result, we have

$$\begin{aligned} N(c^2 + C_3h^2; Q_V^{h,O_0}(a)) &\leq N(c^2 + C_3h^2 + C_6; \frac{1}{4}Q_0^{h,O_0}(0)) \\ &\leq N(C_7; Q_0^{h,O_0}(0)). \end{aligned}$$

It is well-known that there exist $N_0 > 0$ and $C_9 > 0$ such that

$$N(C_7; Q_0^{h,O_0}(0)) \leq C_8h^{-N_0} \quad \text{for } h \in (0, h_0].$$

Hence we have $N((-c, c); P_V^h(a)) = N(c^2; Q_V^h(a)) \leq C_8h^{-N_0}$. □

Under the same situation as in Lemma 2.3, choose $\chi_p \in C_0^\infty(\Omega_p)$ such that $\chi_p = 1$ near U_p and put

$$E_p = [\chi_p v_{p,1}, \ldots, \chi_p v_{p,m_p}], \quad E = \oplus_{p=1}^N E_p$$

and denote the space associated with $\sigma(P_V^h(a)) \cap I(h)$ by F.

Thus we obtain the following proposition.

Proposition 2.6. *Assume that there exists a function $a(h) > 0$ such that $|\log a(h)| = o(1/h)$ as $h \downarrow 0$ and*

$$\begin{aligned} \sigma(P_V^h(a)) \bigcap \{(I(h) + B(0, 2a(h)) \setminus I(h)\} &= \emptyset , \\ \sigma(P_V^{h,\Omega_p}(a)) \bigcap \{(I(h) + B(0, 2a(h)) \setminus I(h)\} &= \emptyset , \end{aligned}$$

for $p = 1, 2, \ldots, N$. Then we have the following:

(i) *There exists $c_1 = c_1(\eta) > 0$ such that $\overrightarrow{d}(E, F) = \overrightarrow{d}(F, E) = O(e^{-c_1/h})$ as $h \downarrow 0$.*

(ii) *There exists a small constant $h_1 > 0$ such that for any $h \in (0, h_1]$, there exists a bijection*

$$b_h : \sigma(P_V^h(a)) \bigcap I(h) \to \bigcup_{p=1}^{N} \sigma(P_V^{h,\Omega_p}(a)) \bigcap I(h)$$

satisfying $|b_h(\lambda) - \lambda| = O(e^{-c_1/h})$ for $\lambda \in \sigma(P_V^h(a)) \cap I(h)$ and $h \in (0, h_1]$.

Proof. Since $d_p(x) \geq c$ on $\mathrm{supp}\,(1 - \chi_p)$ for some constant $c > 0$, Lemma 2.3 leads to

$$(\chi_p v_{p,k}, \chi_p v_{p,l}) = \delta_{kl} + O(e^{-c_1/h}) \quad \text{as} \;\; h \to 0\,,$$

for some $c_1 = c_1(\eta) > 0$. Moreover, we can see that

$$P_V^h(a)(\chi_p v_{p,k}) = \mu_{p,k}\chi_p v_{p,k} - ih(\alpha \cdot \nabla\chi_p)v_{p,k}\,,$$

and $\|ih(\alpha\cdot\nabla\chi_p)v_{p,k}\| = O(e^{-c_1/h})$. Since $M+m_1+m_2+\cdots+m_N = O(h^{-N_0})$ by Proposition 2.5, thus it suffices to apply Proposition 2.4 with $A = P_V^h(a), I = I(h), a = a(h)$. □

Remark 2.7. In Section 3, we shall take $I(h) = [-Ch, Ch]$ and $a(h) = \epsilon h$ for some $C > 0$ and small $\epsilon > 0$. Then we shall see that the eigenvalue problem is reduced to that of the direct sum for the Dirichlet realizations of $P_V^{h,\Omega_p}(a)$ modulo an exponentially error term.

Next, we shall introduce the results which are essentially due to [12] on asymptotic expansion of eigenvalues (see also [2] and [3]).

Let $\mathcal{H}$ be a separable Hilbert space and H_0 a self-adjoint operator on $\mathcal{H}$ with domain $D(H_0)$. Moreover, let $E_0 \in \sigma_{\mathrm{disc}}(H_0)$ and $\mathcal{H}_0$ be the corresponding eigenspace. Assume that there exists a self-adjoint operator H^h on $\mathcal{H}$ with a parameter $h \in (0, h_0]$, sequences $\{H_j\}_{j=1}^{\infty}$, $\{R_j\}_{j=1}^{\infty}$ consisting of symmetric operators with common domain $\mathcal{H}_{\infty}^1$ and there exists a subspace $\mathcal{H}_{\infty}$ of $\mathcal{H}$ such that

$$\mathcal{H}_0 = \mathrm{Ker}(H_0 - E_0) \subset \mathcal{H}_{\infty} \subset \mathcal{H}_{\infty}^1 \subset D(H_0) \cap D(H^h)$$

and

$$\begin{aligned}(H_0 - E_0)^{-1}\overline{\Pi}_{\mathcal{H}_0}(\mathcal{H}_{\infty}) &\subset \mathcal{H}_{\infty},\\ (H_0 - E_0)^{-1}\overline{\Pi}_{\mathcal{H}_0}H_m(\mathcal{H}_{\infty}) &\subset \mathcal{H}_{\infty}.\end{aligned}$$

Here we denote the orthogonal projection onto the orthogonal complement of E by $\overline{\Pi}_E$. Finally, we assume that for any $m \geq 1$, there exists a constant $C_m > 0$ such that

$$\|H^h u - h\sum_{j=0}^{m-1} h^{j/2} H_j u\| \leq C_m h^{(m+2)/2} \|R_m u\| \quad \text{for } u \in \mathcal{H}_\infty.$$

Then we can state a proposition whose proof is found in [2], [3] or [12].

Theorem 2.8. *Addition to the hypotheses as above, suppose that one of the following* (i), (ii) *and* (iii) *holds.*

(i) $\dim \mathcal{H}_0 = 1$.

(ii) $\dim \mathcal{H}_0 > 1$. *There exists an integer* $j_1 > 0$ *such that* $H_l = 0$ *for* $0 < l < j_1$ *and* $K_{j_1} := \Pi_{\mathcal{H}_0} H_{j_1}|_{\mathcal{H}_0}$ *has a non-degenerate eigenvalue* E_{j_1} *with the eigenspace* $\mathcal{H}_{j_1}$.

(iii) $\dim \mathcal{H}_0 > 1$. *There exist integers* j_1, j_2 $(1 \leq j_1 < j_2 \leq 2j_1)$ *such that* $H_l = 0$ *for* $0 < l < j_2$ *and* $l \neq j_1$ *and assume that* K_{j_1} *in* (ii) *has an eigenvalue* E_{j_1} *with the eigenspace* $\mathcal{H}_{j_1}$ *of* $\dim \mathcal{H}_{j_1} > 1$.

Moreover assume that:

$(\text{iii})_1$ *When* $j_2 < 2j_1$, $K_{j_2} := \Pi_{\mathcal{H}_{j_1}} H_{j_2}\Big|_{\mathcal{H}_{j_1}}$ *has a non-degenerate eigenvalue* E_{j_2}.

$(\text{iii})_2$ *When* $j_2 = 2j_1$ *and* $H_{j_1} \not\equiv 0$,

$$K_{j_2} := \Pi_{\mathcal{H}_{j_1}}[-(H_{j_1} - E_{j_1})(H_0 - E_0)^{-1}\overline{\Pi}_{\mathcal{H}_0}(H_{j_1} - E_{j_1}) + H_{j_2}]\Big|_{\mathcal{H}_{j_1}}$$

has a non-degenerate eigenvalue E_{j_2}.

Finally, we assume that there exists $\epsilon_0 > 0$ *such that*

$$\sigma(H^h) \cap I_{\epsilon_0}(h) = \sigma_{\text{disc}}(H^h) \cap I_{\epsilon_0}(h),$$

where $I_{\epsilon_0}(h) = [(E_0 - \epsilon_0)h, (E_0 + \epsilon_0)h]$. *Then* H^h *has a non-degenerate eigenvalue* $\lambda(h)$ *of the form:*

$$\lambda(h) \sim h \sum_{l=0}^{\infty} h^{l/2} E_l, \tag{2.5}$$

where $E_l = 0,\ 0 < l < j_1$ *in the case* (ii) *and* (iii), *and* $E_l = 0,\ j_1 < l < j_2$ *in the case* (iii).

Here the notation $\sim$ *means that for any* $m \geq 1$, *there exists* $C_m > 0$ *such that*

$$\left|\lambda(h) - h\sum_{l=0}^{m-1} h^{l/2} E_l\right| \leq C_m h^{(m+2)/2}, \quad h \in (0, h_0].$$

Now, assume that there exists an operator $J : \mathcal{H} \to \mathcal{H}$ satisfying the following:

$$\begin{cases} J(\lambda u + \mu v) = \overline{\lambda} J(u) + \overline{\mu} J(v), \quad \text{for } \lambda, \mu \in \mathbf{C}, u, v \in \mathcal{H}, \\ J^2(u) = -u, \quad (Ju, u) = 0, \quad \text{for } u \in \mathcal{H}, \\ J(D(H_0)) = D(H_0), \quad J(D(H^h)) = D(H^h), \\ JH_0 = H_0 J, \quad JH^h = H^h J, \\ JH_k(u) = H_k J(u), \quad \text{for } u \in \mathcal{H}_\infty, k \geq 1. \end{cases}$$

We replace the hypotheses (i) $\sim$ (iii) in Theorem 2.8 as follows:

(i) $\dim \mathcal{H}_0 = 2$.

(ii) $\dim \mathcal{H}_0 > 2, \quad \dim \mathcal{H}_{j_1} = 2$.

(iii)$_1$ $\dim \mathcal{H}_0 > 2, \quad \dim \mathcal{H}_{j_1} > 2, \quad \dim \mathcal{H}_{j_2} = 2$.

(iii)$_2$ $\dim \mathcal{H}_0 > 4, \quad \dim \mathcal{H}_{j_1} > 2, \quad \dim \mathcal{H}_{j_2} = 2$.

Then we have the following theorem.

Theorem 2.9. *Under the above situations, H^h has a double eigenvalue $\lambda(h)$ with the eigenspace of the form $[u^h, Ju^h]$ such that $\lambda(h)$ has the asymptotic expansion of the form* (2.5).

3. Eigenvalue Asymptotics in the Case of Point Wells

In this section, we treat the case, where the set U of wells consists of finitely many points. In order to do so, we assume (S.1), (V.1) and

$$-1 \leq V(x) \leq 1 \quad \text{for } x \in \mathbf{R}^3. \tag{V.2}$$

Let $U = \{z_p\}_{p=1}^N = \{x \in \mathbf{R}^3; V(x)^2 = 1\}$ be the set of the electric wells. Thus we can write $U = U^+ \cup U^-$, where $U^\pm = \{x \in \mathbf{R}^3; V(x) = \pm 1\} = \{z_p^\pm\}_{p=1}^{N_\pm}$, $N = N_+ + N_-$. Then we choose regular open neiborhoods $\Omega_p^\pm$ of $z_p^\pm$ as in Section 2. Moreover, assume the non-degeneracy of the Hessian at $z_p^\pm$, i.e.,

$$\pm V''(z_p^\mp) \quad \text{are positively definite.} \tag{V.3}$$

Here we denote the Hessian $((\partial_i \partial_j V)(a))$ of V at $x = a$ by $V''(a)$.

Now, we introduce the Pauli operator which is related to the Dirac operator $P_V^h(a)$. We simply write the skew-symmetric matrix $B(z_p)$ corresponding to the magnetic field at z_p by $B_p = (B_{p,jk})$ and also write

$$V_p'' = \begin{cases} V''(z_p^-) & \text{if } z_p = z_p^-, \\ -V''(z_p^+) & \text{if } z_p = z_p^+. \end{cases}$$

So we note that V_p'' is positively definite. For every $p = 1, 2, \ldots, N$, define an operator

$$H_0^{(p)} = [\sum_{j=1}^{3}(i\partial_j - (B_p x)_j/2)^2 + x \cdot V_p'' x] I_2 + i \sum_{j<k} \sigma_k \sigma_j B_{p,kj} \,, \tag{3.1}$$

on $L^2(\mathbf{R}^3; \mathbf{C}^2)$.

First of all, we examine the spectrum of $H_0^{(p)}$. If we define a skew-symmetric matrix

$$M_p = \begin{bmatrix} B_p & \sqrt{V_p''} \\ -\sqrt{V_p''} & 0 \end{bmatrix},$$

we see that the eigenvalues of M_p are pure imaginary or zero and so we denote them by $\pm i s_{p,j}$ $(0 \le s_{p,1} \le s_{p,2} \le s_{p,3})$. Note that $\Pi_{j=1}^{3}(s_{p,j})^2 = \det(V_p'')$ (cf. Matsumoto and Ueki [10]).

Then we have the following proposition.

Proposition 3.1. *For fixed $p = 1, 2, \ldots, N$, the spectrum of $H_0^{(p)}$ is discrete and*

$$\sigma(H_0^{(p)}) = \{\mu_p^{\pm}(n); n = (n_1, n_2, n_3) \in (\mathbf{Z}_+)^3\} \,, \tag{3.2}$$

where

$$\mu_p^{\pm}(n) = \sum_{j=1}^{3}(2n_j + 1)s_{p,j} \pm |B_p|/\sqrt{2} \quad \text{and} \quad |B_p| = \{\sum_{j,k=1}^{3} B_{p,jk}^2\}^{1/2}.$$

The multiplicities of $\mu_p^{\pm}(n)$ is equal to

$$\#\{n' \in (\mathbf{Z}_+)^3; \mu_p^{\pm}(n') = \mu_p^{\pm}(n)\} + \#\{n' \in (\mathbf{Z}_+)^3; \mu_p^{\mp}(n') = \mu_p^{\pm}(n)\} \,,$$

where $\#A$ denotes the cardinal number for a set A.

Proof. Since $A_p = i\sum_{j<k} \sigma_k \sigma_j B_{p,kj}$ has eigenvalues $\pm|B_p|/\sqrt{2}$, there exists an unitary matrix U_p on $\mathbf{C}^2$ such that

$$(U_p)^* A_p U_p = \begin{bmatrix} -|B_p|/\sqrt{2} & 0 \\ 0 & |B_p|/\sqrt{2} \end{bmatrix}.$$

Therefore, by the unitary transformation, it suffices to consider

$$H_0^{(p)} = H_{00}^{(p)} I_2 + \begin{bmatrix} -|B_p|/\sqrt{2} & 0 \\ 0 & |B_p|/\sqrt{2} \end{bmatrix},$$

where $H_{00}^{(p)} = \sum_{j=1}^{3}(i\partial_j - (B_p x)_j/2)^2 + x \cdot V_p'' x$ on $L^2(\mathbf{R}^3)$. According to [10], we can see that $\sigma(H_{00}^{(p)}) = \sigma_{\mathrm{disc}}(H_{00}^{(p)}) = \{\sum_{j=1}^{3}(2n_j+1)s_{p,j};\ (n_1, n_2, n_3) \in (\mathbf{Z}_+)^3\}$ including multiplicities. This completes the proof. □

Next, we state a lemma on the discrete spectrum of the Dirichlet realization of $P_V^h(a)$.

Lemma 3.2. *Let $\Omega^+, \Omega^- \subset \mathbf{R}^3$ be regular open sets in the sense of Section 2 and assume that*

$$\sup_{x \in \Omega^{\mp}} (\pm V(x)) < 1.$$

If we put $0 < c^{\mp} := \min\{1, 1 - \sup_{x \in \Omega^{\mp}}(\pm V(x))\} \leq 1$, then we have

$$\begin{aligned} \sigma(P_V^{h,\Omega^-}(a)) \cap (-c^-, 0] &= \emptyset, \\ \sigma(P_V^{h,\Omega^+}(a)) \cap [0, c^+) &= \emptyset. \end{aligned}$$

Proof. We only prove this lemma in the case $\Omega = \Omega^-$ and $c = c^-$. The case, where $\Omega = \Omega^+$ and $c = c^+$, can be treated by the same arguments. Assume that there exists an eigenvalue $E(h) \in \sigma(P_V^{h,\Omega}(a)) \cap (-c, 0]$. If we write the corresponding normalized eigenfunction by $u^h = (u_+^h, u_-^h) \in L^2(\Omega; \mathbf{C}^2) \otimes L^2(\Omega; \mathbf{C}^2)$, then the equation $P_V^{h,\Omega}(a)u^h = E(h)u^h$ is equivalent to

$$\left\{ \begin{array}{l} (1 + V - E(h))u_+^h + \sigma \cdot D^h(a)u_-^h = 0, \\ (-1 + V - E(h))u_-^h + \sigma \cdot D^h(a)u_+^h = 0. \end{array} \right. \tag{3.3}$$

Therefore, we have

$$\begin{aligned} ((1 + V - E(h))u_+^h, u_+^h) \quad - \quad & ((-1 + V - E(h))u_-^h, u_-^h) \\ & = 2i \operatorname{Im}(\sigma \cdot D^h(a)u_-^h, u_+^h). \end{aligned}$$

Taking the real part of the both hand sides, we have

$$((1 + V - E(h))u_+^h, u_+^h) - ((-1 + V - E(h))u_-^h, u_-^h) = 0.$$

Since $-1 \leq V(x) < 1 - c$ in Ω by the hypothesis, we see that

$$\left\{ \begin{array}{l} ((V - E(h))u_+^h, u_+^h) \geq (-1 - E(h))\|u_+^h\|^2, \\ ((V - E(h))u_-^h, u_-^h) \leq (1 - c - E(h))\|u_-^h\|^2. \end{array} \right.$$

Thus we have

$$\begin{aligned} 0 &= 1 + ((V - E(h))u_+^h, u_+^h) - ((V - E(h))u_-^h, u_-^h) \\ &\geq (c + E(h))\|u_-^h\|^2 - E(h)\|u_+^h\|^2. \end{aligned} \tag{3.4}$$

Since $c + E(h) > 0$ and $E(h) \le 0$, we get $u^h_- = 0$. If $E(h) < 0$, (3.4) leads to $u^h_+ = 0$. If $E(h) = 0$, it follows from (3.3) that $(1 + V(x))u^h_+ = 0$. Therefore, we see $u^h_+ = 0$ by the hypothesis (V.3). Thus, we reach the contradiction. □

By the Taylor expansions of V and a at $x = z^\pm_p$ and a gauge transformation, we may write

$$\begin{aligned} a_j(x) &= -(B_p\,(x - z^\pm_p))_j/2 + O(|x - z^\pm_p|^2)\,, \\ V(x) &= \mp 1 + \tfrac{1}{2}(x - z^\pm_p)\cdot V''_p\,(x - z^\pm_p) + O(|x - z^\pm_p|^3)\,, \end{aligned} \tag{3.5}$$

as $x \to z^\pm_p$. Taking Lemma 3.2 into consideration, let

$$0 < \pm\lambda^\pm_{p,1}(h) \le \pm\lambda^\pm_{p,2}(h) \le \cdots$$

be the sequence of the eigenvalues of $P^{h,\Omega^\mp_p}_V(a)$ in $(0,1)$ or $(-1,0)$ and $\{e^\pm_{p,k}\}_{k=1}^\infty$ be the increasing sequence of the eigenvalues of $H^{(p)}_0$ for $z_p = z^\pm_p$ on $L^2(\mathbf{R}^3;\mathbf{C}^2)$.

Then we can get the first main theorem on an estimate for the eigenvalues $\lambda^\pm_{p,k}(h)$.

Theorem 3.3. *For every $p = 1, 2, \ldots, N$ and $k > 0$, there exists a constant $C_{p,k} > 0$ such that*

$$|\lambda^\pm_{p,k}(h) - \frac{1}{2}he^\pm_{p,k}| \le C_{p,k}h^{3/2} \quad \text{for } \ h \in (0, h_0]. \tag{3.6}$$

Proof. At the first time, we prove the case, where $z_p = z^-_p$ and simply write $\Omega = \Omega^-_p$. Let $\lambda(h) \in (0,1)$ be an eigenvalue of $P^{h,\Omega}_V(a)$ and u^h an associated normalized eigenfunction. We write u^h in the form: $u^h = (u^h_+, u^h_-) \in L^2(\mathbf{R}^3;\mathbf{C}^2) \otimes L^2(\mathbf{R}^3;\mathbf{C}^2)$. Since we can choose Ω as a small neighborhood of z_p, we may assume that $V(x) - \lambda(h) \le V(x) < 0$ in Ω. Then the equation $P^{h,\Omega}_V(a)u^h = \lambda(h)u^h$ is equivalent to

$$\begin{cases} \sigma\cdot D^h(a)u^h_- + (1 + V(x) - \lambda(h))u^h_+ = 0\,, \\ \sigma\cdot D^h(a)u^h_+ + (-1 + V(x) - \lambda(h))u^h_- = 0\,. \end{cases}$$

That is to say,

$$\begin{cases} \big[\sigma\cdot D^h(a)\big(1 - (V(x) - \lambda(h))\big)^{-1}\sigma\cdot D^h(a) \\ \quad +(1 + V(x) - \lambda(h))\big]u^h_+ = 0, \\ u^h_- = (1 - (V(x) - \lambda(h)))^{-1}\sigma\cdot D^h(a)u^h_+. \end{cases} \tag{3.7}$$

Choose $\chi \in C_0^\infty(\Omega)$ such that $\chi = 1$ near $x = z_p$. By Lemma 2.3, we see that there exist positive constants C_1 and c_1 such that

$$\|(P_V^h(a) - \lambda(h))\chi u^h\| \le C_1 e^{-c_1/h},$$
$$\|\chi u^h - u^h\| \le C_1 e^{-c_1/h}.$$

Thus if we choose $\chi_1 \in C_0^\infty(\Omega)$ such that $\chi_1 = 1$ on $\operatorname{supp}\chi$, we have

$$(P_{\chi_1 V}^h(\chi_1 a) - \lambda(h))\chi u^h = (P_V^h(a) - \lambda(h))\chi u^h.$$

Therefore, we may assume that $\operatorname{supp} V$ and $\operatorname{supp} a$ are contained in Ω.

If we put $v_+^h = \big(1-(V(x)-\lambda(h))\big)^{-1/2}\chi u_+^h$, we can rewrite the first equation in (3.7) in the form $H^h(a, V, \lambda(h))v_+^h = O(e^{-c_1/h})$, where

$$\begin{aligned} &H^h(a, V, \lambda(h)) \\ &\quad = \big[D^h(a)^2 + h^2\big\{\tfrac{3}{4}(\nabla V(x)\cdot\nabla V(x))\big(1-(V(x)-\lambda(h))\big)^{-2} \\ &\qquad +\tfrac{1}{2}(\Delta V(x))\big(1-(V(x)-\lambda(h))\big)^{-1}\big\} + 1 - (V(x)-\lambda(h))^2\big]I_2 \\ &\qquad + ih\textstyle\sum_{j<k}\sigma_k\sigma_j B_{kj}(x). \end{aligned} \tag{3.8}$$

Using (3.5), we may write

$$H^h(a, V, \lambda(h))v_+^h = (\widetilde{H}_0^{(p)}(h) - 2\lambda(h))v_+^h + R^{(p)}(h)v_+^h\,, \tag{3.9}$$

where

$$\begin{aligned} \widetilde{H}_0^{(p)}(h) = \big[&\textstyle\sum_{j=1}^3 (ih\partial_j - (B_p(x-z_p))_j/2)^2 \\ &+(x-z_p)\cdot V_p''(x-z_p)\big]I_2 + ih\textstyle\sum_{j<k}\sigma_k\sigma_j B_{p,kj}. \end{aligned} \tag{3.10}$$

If we define a unitary operator U_h^p on $L^2(\mathbf{R}^3;\mathbf{C}^2)$:

$$(U_h^p f)(x) = h^{-3/4} f(h^{-1/2}(x - z_p)) \quad \text{for } f \in L^2(\mathbf{R}^3;\mathbf{C}^2), \tag{3.11}$$

then we can write

$$(U_h^p)^* H^h(a, V, \lambda(h)) U_h^p = hH_0^{(p)} - 2\lambda(h) + (U_h^p)^* R^{(p)}(h) U_h^p\,,$$

where $H_0^{(p)}$ is as in (3.1) and we have

$$\|(U_h^p)^* R^{(p)}(h) U_h^p w_+^h\| \le C_1 h^{3/2} \|w_+^h\|\,,$$

with $w_+^h = (U_h^p)^* v_+^h$ for $h \in (0, h_0]$.

Thus we have

$$\|(hH_0^{(p)} - 2\lambda(h))w_+^h\| \le C_1 h^{3/2}\|w_+^h\|. \tag{3.12}$$

In order to apply Proposition 2.4, let $\lambda(h)$ be an eigenvalue of $P_V^{h,\Omega_p}(a)$ with multiplicity m and $u_j^h = (u_{j,+}^h, u_{j,-}^h)$ $(j = 1, 2, \dots, m)$ the basis of the eigenspace consisting of normalized eigenfunctions. As above, if we define $v_{j,+}^h = \big(1 - (V(x) - \lambda(h)\big)^{-1/2}\chi u_{j,+}^h$ and $w_{j,+}^h = (U_h^p)^* v_{j,+}^h$, then it follows from (3.12) that

$$\|(hH_0^{(p)} - 2\lambda(h))w_{j,+}^h\| < C_1 h^{3/2}\|w_{j,+}^h\|.$$

We can also see that $\{w_{j,+}^h\}_{j=1,2,\dots,m}$ are linearly independent. Put $I(h) = [2\lambda(h) - C_1 h^{3/2}, 2\lambda(h) + C_1 h^{3/2}]$, $E = [w_{1,+}^h, \dots, w_{m,+}^h]$ the subspace spanned by $w_{j,+}^h$ $(j = 1, 2, \dots, m)$ and F the space associated to $\sigma(hH_0^{(p)}) \cap I(h)$ as in Proposition 2.4. If we choose $\epsilon > 0$ small enough, we can see that

$$\sigma(hH_0^{(p)}) \cap ((I(h) + B(0, 2\epsilon h) \setminus I(h)) = \emptyset.$$

Therefore it follows from Proposition 2.4 that $\overrightarrow{d}(E, F) \le C_\epsilon h^{1/2}$. Thus, for small $h > 0$, $hH_0^{(p)}$ has at least m eigenvalues in $I(h)$.

Conversely, let e be an eigenvalue of $H_0^{(p)}$ with multiplicity m_0 and write the basis of the corresponding eigenspace consisting of normalized eigenfunctions by w_j $(j = 1, \dots, m_0)$. As above, we define $v_{j,+}^h = U_h^p w_{j,+}^h$, $u_{j,+}^h = \big(1 - (V(x) - he)\big)^{1/2} v_{j,+}^h$ and define functions $u_{j,-}^h$ by the second equality in (3.7) and put $u_j^h = (u_{j,+}^h, u_{j,-}^h)$. Then we can see that $\|\chi u_j^h - u_j^h\| \le C_2 e^{-c_1/h}\|u_j^h\|$ and we have

$$\|(P_V^{h,\Omega}(a) - \frac{1}{2}he)\chi u_j^h\| \le C_2 h^{3/2}\|u_j^h\|.$$

It is easily seen that $\{u_j^h\}_{j=1,2,\dots,m_0}$ are linearly independent. Put

$$I(h) = [\frac{1}{2}he - C_2 h^{3/2}, \frac{1}{2}he + C_2 h^{3/2}],$$

$E = [u_1^h, \dots, u_{m_0}^h]$, F the space associated to $\sigma(P_V^{(h,\Omega}(a)) \cap I(h)$ as in Proposition 2.4. If we choose $\epsilon > 0$ small enough, we also can see that

$$\sigma(P_V^{h,\Omega}(a)) \cap ((I(h) + B(0, 2\epsilon h) \setminus I(h)) = \emptyset.$$

Thus we also see that $\overrightarrow{d}(E, F) \le C_\epsilon h^{1/2}$. Therefore, for small $h > 0$, $P_V^{h,\Omega}(a)$ has at least m_0 eigenvalues in $I(h)$. From these facts, we get to the conclusion in the case $\Omega = \Omega_p^-$.

Similarly, in the case $\Omega = \Omega_p^+$, let $0 > \lambda_{p,1}^-(h) \geq \lambda_{p,2}^-(h) \geq \cdots$ be a decreasing sequence of the eigenvalues of $P_V^{h,\Omega_p^+}(a)$ in $(-1,0)$ and $\{e_{p,k}^-\}_{k=1}^\infty$ be a increasing sequence of the eigenvalues of $H_0^{(p)}$ on $L^2(\mathbf{R}^3;\mathbf{C}^2)$. Then we have

$$\lambda_{p,k}^-(h) = \frac{1}{2}he_{p,k}^- + O(h^{3/2}) \quad \text{as } h \downarrow 0.$$

This completes the proof. □

Finally, we remark that if we take $I(h) = [-Ch, Ch]$ for some $C > 0$ and $a(h) = \epsilon h$ for small $\epsilon > 0$, it follows from Proposition 2.6 that there exist $h_1 > 0$, $c_1 > 0$ and bijections

$$b_h : \sigma(P_V^h(a)) \cap I(h) \to \bigcup_{p=1}^{N} \sigma(P_V^{h,\Omega_p}(a)) \cap I(h)$$

satisfying $|b(\lambda) - \lambda| = O(e^{-c_1/h})$ for all $\lambda \in \sigma(P_V^h(a))$ and $h \in (0, h_1]$.

4. Asymptotics of Some Eigenvalues

In this section, we want to get the complete asymptotic expansion of some eigenvalue $\lambda(h)$ of $P_V^h(a)$.

Throughout this section, we assume that (S.1) and (V.1) $\sim$ (V.3) hold. By the Taylor expansions of $a(x)$ and $V(x)$ at $x = z_p = z_p^\pm$, we have

$$\begin{aligned} a_j(x) &= \sum_{l=0}^{N-1} a_{p,j}^{(l)}(x - z_p) + \widehat{a}_{p,j}^{(N)}(x - z_p), \\ B_{kj}(x) &= \sum_{l=0}^{N-1} B_{p,kj}^{(l)}(x - z_p) + \widehat{B}_{p,kj}^{(N)}(x - z_p), \\ V(x) &= \pm 1 \mp \frac{1}{2}(x - z_p^\pm) \cdot V''(z_p^\pm)(x - z_p^\pm) + \sum_{l=3}^{N-1} V_p^{(l)}(x - z_p) \\ &\quad + \widehat{V}_p^{(N)}(x - z_p)\,, \end{aligned} \tag{4.1}$$

where

$$\begin{aligned} a^{(l)}_{p,j}(x) &= \sum_{|\alpha|=l} \frac{x^\alpha}{\alpha!}(\partial^\alpha a_j)(z_p) \quad (l \geq 0), \quad \widehat{a}^{(N)}_{p,j}(x) = O(|x|^N), \\ B^{(l)}_{p,kj}(x) &= \sum_{|\alpha|=l} \frac{x^\alpha}{\alpha!}(\partial^\alpha B_{kj})(z_p) \quad (l \geq 0), \quad \widehat{B}^{(N)}_{p,kj}(x) = O(|x|^N), \\ V^{(l)}_p(x) &= \sum_{|\alpha|=l} \frac{x^\alpha}{\alpha!}(\partial^\alpha V)(z_p) \quad (l \geq 3), \quad \widehat{V}^{(N)}_p(x) = O(|x|^N)\,, \end{aligned}$$

as $|x| \to 0$.

Under the hypothesis (V.3), it is well-known that we can choose a coordinate in $\mathbf{R}^3$ such that $V''_p(z^\pm_p)$ is of the form:

$$V''_p = \mp V''(z^\pm_p) = \begin{bmatrix} \mu_{p,1} & 0 & 0 \\ 0 & \mu_{p,2} & 0 \\ 0 & 0 & \mu_{p,3} \end{bmatrix} \quad (\mu_{p,j} > 0). \tag{V.3'}$$

For brevity of notation, from now on, we assume (V.3)' rather than (V.3).

Choose $\chi_p \in C^\infty_0(\Omega_p)$ such that $\chi_p = 1$ in a small neighborhood of $x = z_p$. Then as seen in Section 3, the eigenvalue problem for $P^h_V(a)$ is reduced to that of $P^{h,\Omega_1}_V(a) \otimes \cdots \otimes P^{h,\Omega_N}_V(a)$ on $L^2(\Omega_1;\mathbf{C}^4) \otimes \cdots \otimes L^2(\Omega_N;\mathbf{C}^4)$ and moreover, for every p, the eigenvalue problem of $P^{h,\Omega_p}_V(a)$ is also reduced to that of $H^{p,h} = H^h(\chi_p a, \chi_p V, \lambda_p(h))$ on $L^2(\mathbf{R}^3;\mathbf{C}^2)$. Thus, it suffices to consider

$$H^{p,h}(\chi_p a, \chi_p V, \lambda_p(h)) u^h = 0 \quad \text{on} \quad L^2(\mathbf{R}^3;\mathbf{C}^2)\,,$$

for every $p = 1, 2, \ldots, N$. We search for the eigenvalue $\lambda_p(h)$ of $P^h_V(a)$ of the form $\lambda_p(h) \sim h \sum_{l=0}^\infty h^{l/2} E_{p,l}$.

If we apply the Taylor expansion (4.1) to (3.8) and use the unitary transformation (3.11), we can write, for any $m \geq 1$,

$$\widetilde{H}^{p,h} := (U^p_h)^* H^{p,h} U^p_h = h \sum_{l=0}^{m-1} h^{l/2}(H^{(p)}_l - 2E_{p,l}) + R^h_m(a, V, \lambda_p(h))\,, \tag{4.2}$$

where

$$\begin{aligned} H^{(p)}_0 &= \left[(D(B^{(0)}_p))^2 + 2V^{(2)}\right] I_2 + i \sum_{j<k} \sigma_k \sigma_j B^{(0)}_{p,kj}, \\ H^{(p)}_l &= \left[D(B^{(0)}_p) \cdot a^{(l+1)}_p(x) + a^{(l+1)}_p(x) \cdot D(B^{(0)}_p) + Q_{p,l}(x)\right] I_2 \\ &\quad + i \sum_{j<k} \sigma_k \sigma_j B^{(l)}_{p,kj}(x) \quad (l \geq 1). \end{aligned}$$

Here we denote

$$\begin{aligned} D(B_p^{(0)}) &= (D_1(B_p^{(0)}), D_2(B_p^{(0)}), D_3(B_p^{(0)})), D_j(B_p^{(0)}) \\ &= i\partial_j - (B(z_p)\,x)_j/2, \end{aligned}$$

$Q_{p,l}(x)$ is a real polynomial of degree $l+2$ depending only on $E_{p,k}$ $(k \le l-2)$ and $R_m^h(a, V, \lambda_p(h))$ satisfies that

$$\|R_m^h(a, V, \lambda_p(h))u\| \le Ch^{(m+2)/2}\|u\| \quad \text{for} \quad u \in C_0^\infty(\mathbf{R}^2; \mathbf{C}^2).$$

Since we need the concrete representations of $Q_{p,l}$ for $l \le 4$ later, we list them here.

$$\begin{aligned} Q_{p,1} &= 2V_p^{(3)}, \\ Q_{p,2} &= a_p^{(2)} \cdot a_p^{(2)} + 2V_p^{(4)} + \tfrac{1}{4}\textstyle\sum_{j=1}^3 \mu_{p,j} + (V_p^{(2)} - E_{p,0})^2, \\ Q_{p,3} &= 2a_p^{(2)} \cdot a_p^{(3)} + 2^{-2}\Delta V_p^{(3)} + 2V_p^{(5)} + 2(V_p^{(2)} - E_{p,0})(V_p^{(3)} - E_{p,1}), \\ Q_{p,4} &= 2a_p^{(2)} \cdot a_p^{(4)} + a_p^{(3)} \cdot a_p^{(3)} + 2^{-4} \cdot 3\nabla V_p^{(2)} \cdot \nabla V_p^{(2)} \\ &\quad +2^{-3}\Delta V_p^{(2)}(V_p^{(2)} - E_{p,0}) + 2^{-2}\Delta V_p^{(4)} + 2V_p^{(6)} \\ &\quad +2(V_p^{(2)} - E_{p,0})(V_p^{(4)} - E_{p,2}) + (V_p^{(3)} - E_{p,1})^2. \end{aligned} \tag{4.3}$$

For brevity of the notations, we use the following symbols.

$$\begin{aligned} \partial_{p,\mu} &= (\partial_{p,\mu,1}, \partial_{p,\mu,2}, \partial_{p,\mu,3}) = (\mu_{p,1}^{-1/4}\partial_1, \mu_{p,2}^{-1/4}\partial_2, \mu_{p,3}^{-1/4}\partial_3), \\ \partial_{p,\mu}^\alpha &= \partial_{p,\mu,1}^{\alpha_1}\partial_{p,\mu,2}^{\alpha_2}\partial_{p,\mu,3}^{\alpha_3} \quad \text{for} \ \ \alpha = (\alpha_1, \alpha_2, \alpha_3) \in (\mathbf{Z}_+)^3, \\ \Delta_{p,\mu} &= \partial_{p,\mu} \cdot \partial_{p,\mu} = \mu_{p,1}^{-1/2}\partial_1^2 + \mu_{p,2}^{-1/2}\partial_2^2 + \mu_{p,3}^{-1/2}\partial_3^2. \end{aligned} \tag{4.4}$$

Now we are in a position to state the main theorem in this section.

Theorem 4.1. *We assume that* (S.1), (V.1), (V.2) *and* (V.3)$'$ *hold.*

(i) *Assume that $B(z_p) \neq 0$ for some $p = 1, 2, \ldots, N$. Then $P_V^h(a)$ has an eigenvalue $\lambda_p(h)$ of the form*

$$\lambda_p(h) \sim h\sum_{l=0}^\infty h^{l/2}E_{p,l}\,, \tag{4.5}$$

where $E_{p,0} = \frac{1}{2}\sum_{j=1}^3 s_{p,j} - \frac{1}{2\sqrt{2}}|B(z_p)|$ and $s_{p,j}$ are as in Proposition 3.1.

(ii) *Assume that $B(z_p) = 0$ and*

$$\sum_{i<j}\Big[\sum_{k=1}^3 \mu_{p,k}^{-1/2}(\partial_{p,\mu,k}\Delta_{p,\mu}V)(z_p) \cdot (\partial_{p,\mu,k}B_{ij})(z_p) - (\Delta_{p,\mu}B_{ij})(z_p)\Big]^2 \neq 0\,, \tag{4.6}$$

for some $p = 1, 2, \dots, N$*. Let* $\mathcal{H}_0$ *be the eigenspace of* $H_0^{(p)}$ *corresponding to the ground state energy* $2E_{p,0} = \sum_{j=1}^{3} \sqrt{\mu_{p,j}}$*. Then* $\Pi_{\mathcal{H}_0}[H_1^{(p)}]|_{\mathcal{H}_0}$ *has a double eigenvalue* $2E_{p,1}$ *with the corresponding eigenspace* $\mathcal{H}_1 = \mathcal{H}_0$ *and*

$$K_2 := \Pi_{\mathcal{H}_0}\big[-H_1^{(p)}(H_0^{(p)} - 2E_{p,0})^{-1}\overline{\Pi}_{\mathcal{H}_0}H_1^{(p)} + H_2^{(p)}\big]\big|_{\mathcal{H}_0}$$

has two simple eigenvalues $2E_{p,2,1} < 2E_{p,2,2}$*. Moreover,* $P_V^h(a)$ *has two eigenvalues* $\lambda_{p,i}(h)$ $(i = 1, 2)$ *of the form*

$$\lambda_{p,i}(h) \sim h\big(E_{p,0} + h^{1/2}E_{p,1} + hE_{p,2,i} + \sum_{l=3}^{\infty} h^{l/2}E_{p,l,i}\big) \quad (i = 1, 2)\,, \tag{4.7}$$

as $h \to 0$*. In the particular case where* $(\partial^\alpha V)(z_p) = 0$ *for* $|\alpha| = 3$ *and* $(\partial^\alpha a)(z_p) = 0$ *for* $|\alpha| = 2$*, we can see that* (4.6) *becomes*

$$\sum_{i<j}[(\Delta_{p,\mu}B_{ij})(z_p)]^2 \neq 0\,,$$

which is equivalent to $\sum_{i<j}[(\Delta B_{ij})(z_p)]^2 \neq 0$ *and we can put* $E_{p,1} = 0$ *in* (4.7).

(iii) *Assume that for some* $p = 1, 2, \dots, N$, $(\partial^\alpha a)(z_p) = 0$ *for* $|\alpha| = 2$, 4 *and* $(\partial^\alpha V)(z_p) = 0$ *for* $|\alpha| = 3$, 5*. Moreover, assume that the left hand side of* (4.6) *vanishes and*

$$\begin{aligned}\sum_{i<j}\Big[\sum_{k,l=1}^{3} &\frac{2}{\sqrt{\mu_{p,k}} + \sqrt{\mu_{p,l}}}(\partial_{p,\mu,k}\partial_{p,\mu,l}\Delta_{p,\mu}V)(z_p)\cdot(\partial_{p,\mu,k}\partial_{p,\mu,l}B_{ij})(z_p)\\ &+ \sum_{k=1}^{3}\mu_{p,k}^{1/2}(\partial_{p,\mu,k}^2 B_{ij})(z_p) - \sum_{k\neq l}\mu_{p,k}^{1/2}(\partial_{p,\mu,l}^2 B_{ij})(z_p)\\ &-(\Delta_{p,\mu}B_{ij})(z_p)\Big]^2 \neq 0.\end{aligned} \tag{4.8}$$

Let $\mathcal{H}_0$ *be an eigenspace of* $H_0^{(p)}$ *corresponding to the ground state energy* $E_{p,0}$ *as in (ii). Then* K_2 *as in (ii) has a double eigenvalue* $2E_{p,2}$ *and we see that*

$$K_4 := \Pi_{\mathcal{H}_0}\big[-H_2^{(p)}(H_0^{(p)} - 2E_{p,0})^{-1}\overline{\Pi}_{\mathcal{H}_0}H_2^{(p)} + H_4^{(p)}\big|_{\mathcal{H}_0}$$

has two simple eigenvalues $2E_{p,4,1} < 2E_{p,4,2}$*. Furthermore* $P_V^h(a)$ *has two eigenvalues* $\lambda_{p,i}(h)$ $(i = 1, 2)$ *of the form*

$$\lambda_{p,i}(h) \sim h\big(E_{p,0} + hE_{p,2} + h^2E_{p,4,i} + \sum_{l=5}^{\infty} h^{l/2}E_{p,l,i}\big) \quad (i = 1, 2)\,, \tag{4.9}$$

as $h \to 0$.

Remark 4.2. (1) Although the calculations of the values of $E_{p,i}$ and $E_{p,i,j}$ above are elementary, they are so long. For this reason, we only calculate them in an example in the next section. The left hand sides in (4.6) and (4.8) are equal to the discriminants of representation matrices of K_2 and K_4 modulo constant times. We shall show these in Appendix.

(2) For all cases, the eigenvalues $\lambda_p(h)$ in the case (i) and $\lambda_{p,i}(h)$ in the case (ii) and (iii) are simple eigenvalues of $P_V^{h,\Omega_p}(a)$ for fixed p. Therefore, in the case of a single well, i.e., $N = 1$, the eigenvalues in the above theorem are non-degenerate (cf. [2], [12]).

Proof of Theorem 4.1. Fix p in the hypotheses of (i), (ii) and (iii). By the arguments in the beginning of this section, it suffices to consider $\widetilde{H}^{p,h}$ in (4.2). By a translation, we may assume that $z_p = 0$ and from now on, we omit the index p for brevity of the notation. According to Proposition 3.1, we have

$$\sigma(H_0) = \sigma_{\text{disc}}(H_0) = \{\mu^{\pm}(n); n \in (\mathbf{Z}_+)^3\}.$$

In order to apply Theorem 2.8, we note that we can take $\mathcal{H}_\infty = \mathcal{H}_\infty^1 = \mathcal{S}(\mathbf{R}^3; \mathbf{C}^2)$ which denote the space of all rapidly decreasing, smooth functions with values in $\mathbf{C}^2$ in Theorem 2.8.

Now we prove (i). In this case, the ground state energy of H_0 is equal to

$$2E_0 = \mu^-(0) = \sum_{j=1}^{3} s_j - |B(0)|/\sqrt{2}\,,$$

which is non-degenerate and the corresponding eigenspace is of the form $\mathcal{H}_0 = \left[\ \phi_0(x)\ \right]$, where $\phi_0(x) = ce^{-\langle x, Xx\rangle}/2$, X is a symmetric matrix such that ReX is positively definite (cf. [10]) and c is the normalized constant. Hence we see that all the hypotheses of Theorem 2.8 (i) hold. Therefore, it is seen that $P_V^h(a)$ has an non-degenerate eigenvalue $\lambda_0(h)$ with the complete expansion of the form

$$\lambda_0(h) \sim h \sum_{l=0}^{\infty} h^{l/2} E_l\,,$$

where $E_0 = \frac{1}{2}\sum_{j=1}^{3} s_j - \frac{1}{2\sqrt{2}}|B(z_p)|$.

For the proofs of (ii) and (iii), we can write $H_0 = H_{00}I_2$, where $H_{00} = -\Delta + \sum_{j=1}^{3}\mu_j x_j^2$ on $L^2(\mathbf{R}^3)$. It is well-known that the spectrum of the harmonic oscillator H_{00} is discrete and $\sigma(H_{00}) = \{\mu_\alpha := \sum_{j=1}^{3}\sqrt{\mu_j}(2\alpha_j + 1); \alpha = (\alpha_1, \alpha_2, \alpha_3) \in (\mathbf{Z}_+)^3\}$. We denote the corresponding normalized eigenfunction to μ_α by $\phi_\alpha(x)$. Thus we see that the ground state energy of H_0 is equal to

$2E_0 = \sum_{j=1}^3 \sqrt{\mu_j}$ which is a double eigenvalue and the corresponding eigenfunctions are

$$\phi_0^+ = \begin{bmatrix} \phi_0 \\ 0 \end{bmatrix}, \quad \phi_0^- = \begin{bmatrix} 0 \\ \phi_0 \end{bmatrix},$$

where $\phi_0(x) = \phi_{(0,0,0)} = ce^{-\sqrt{\mu_j}x_j^2/2}, c = \pi^{-3/4}(\mu_1\mu_2\mu_3)^{1/4}$. Let $\mathcal{H}_0 = [\phi_0^+, \phi_0^-]$ which can be identified with $\mathcal{H}_{00} \oplus \mathcal{H}_{00}$, where $\mathcal{H}_{00} = [\phi_0]$ in $L^2(\mathbf{R}^3)$. In order to apply Theorem 2.8 (iii) with $j_1 = l, j_2 = 2l$ ($l = 1$ or 2), we write

$$H_l = H_{l0}I_2 + \widetilde{B}^{(l)}(x) = (A_{l0} + Q_l)I_2 + \widetilde{B}^{(l)}(x) \quad (l \geq 1),$$

where

$$\begin{aligned} \widetilde{B}^{(l)}(x) &= \begin{bmatrix} \widetilde{B}_{11}^{(l)}(x) & \widetilde{B}_{12}^{(l)}(x) \\ \widetilde{B}_{21}^{(l)}(x) & \widetilde{B}_{22}^{(l)}(x) \end{bmatrix} \\ &= \begin{bmatrix} -B_{12}^{(l)}(x) & -B_{23}^{(l)}(x) - iB_{13}^{(l)}(x) \\ -B_{23}^{(l)}(x) + iB_{13}^{(l)}(x) & B_{12}^{(l)}(x) \end{bmatrix} \\ A_{l0} &= i\sum_{j=1}^3 \big(\partial_j a_j^{(l+1)}(x) + a_j^{(l+1)}(x)\partial_j\big). \end{aligned}$$

In the sequel, we have to consider the representation matrix $M^{(2l)}$ of

$$K_{2l} = \Pi_{\mathcal{H}_0}[-H_l(H_0 - 2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_0}H_l + H_{2l}]\big|_{\mathcal{H}_0},$$

with respect to the basis ϕ_0^+, ϕ_0^- of $\mathcal{H}_0$. In order to do so, we write it by

$$M^{(2l)} = \begin{bmatrix} M_{11}^{(2l)} & M_{12}^{(2l)} \\ M_{21}^{(2l)} & M_{22}^{(2l)} \end{bmatrix} \quad (l = 1, 2).$$

Using the fact that ϕ_0 is a real and even function with respect to x_1, x_2, x_3, the components are computed as follows.

$$
\begin{aligned}
M_{11}^{(2l)} &= -\big((H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}}A_{l0}\phi_0, A_{l0}\phi_0\big)\\
&\quad -\big((H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}}Q_l\phi_0, Q_l\phi_0\big)\\
&\quad +2\big(((H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}}Q_l\phi_0, B_{12}^{(l)}\phi_0\big)\\
&\quad -\textstyle\sum_{i<j}\big(((H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}}B_{ij}^{(l)}\phi_0, B_{ij}^{(l)}\phi_0\big)\\
&\quad +(Q_{2l}\phi_0,\phi_0)-(B_{12}^{(2l)}\phi_0,\phi_0),\\
M_{12}^{(2l)} &= \overline{M_{21}^{(2l)}} = 2\big((H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}}Q_l\phi_0, B_{23}^{(l)}\phi_0\big)\\
&\quad -2i\big((H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}}Q_l\phi_0, B_{13}^{(l)}\phi_0\big)\\
&\quad -(B_{23}^{(2l)}\phi_0,\phi_0)+i(B_{13}^{(2l)}\phi_0,\phi_0),\\
M_{22}^{(2l)} &= -\big((H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}}A_{l0}\phi_0, A_{l0}\phi_0\big)\\
&\quad -\big((H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}}Q_l\phi_0, Q_l\phi_0\big)\\
&\quad -2\big(((H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}}Q_l\phi_0, B_{12}^{(l)}\phi_0\big)\\
&\quad -\textstyle\sum_{i<j}\big(((H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}}B_{ij}^{(l)}\phi_0, B_{ij}^{(l)}\phi_0\big)\\
&\quad +(Q_{2l}\phi_0,\phi_0)+(B_{12}^{(2l)}\phi_0,\phi_0).
\end{aligned}
\tag{4.10}
$$

Then the discriminant $D^{(2l)}$ of the characteristic equation of $M^{(2l)}$ is

$$
\begin{aligned}
D^{(2l)} &= (M_{11}^{(2l)}-M_{22}^{(2l)})^2+4M_{12}^{(2l)}M_{21}^{(2l)}\\
&= 2^2\textstyle\sum_{i<j}\big[2\big((H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}}Q_l\phi_0, B_{ij}^{(l)}\phi_0\big)-(B_{ij}^{(2l)}\phi_0,\phi_0)\big]^2
\end{aligned}
\tag{4.11}
$$

and the eigenvalues $2E_{2l,1}$ and $2E_{2l,2}$ of $M^{(2l)}$ are $2E_{2l,1}=2E_{2l,-}$ and $2E_{2l,2}=2E_{2l,+}$, where

$$
\begin{aligned}
2E_{2l,\mp} &= \frac{M_{11}^{(2l)}+M_{22}^{(2l)}\mp\sqrt{D^{(2l)}}}{2}\\
&= -\big((H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}}A_{l0}\phi_0, A_{l0}\phi_0\big)\\
&\quad -\big((H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}}Q_l\phi_0, Q_l\phi_0\big)\\
&\quad -\textstyle\sum_{i<j}\big((H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}}B_{ij}^{(l)}\phi_0, B_{ij}^{(l)}\phi_0\big)\\
&\quad +(Q_{2l}\phi_0,\phi_0)\mp 2^{-1}\sqrt{D^{(2l)}}.
\end{aligned}
\tag{4.12}
$$

Now we prove (ii). We apply Theorem 2.8 (iii) with $j_1=1, j_2=2$. Since ϕ_0 is a real and even function, we have $(B_{ij}^{(1)}\phi_0,\phi_0)=0$ and $(H_{10}\phi_0,\phi_0)=0$. Thus $\Pi_{\mathcal{H}_0}H_1\big|_{\mathcal{H}_0}$ has a double eigenvalue $E_1=0$. Of course, the corresponding eigenspace is equal to $\mathcal{H}_0$. After a computation of $D^{(2)}$, we have

$$\begin{aligned} D^{(2)} &= 2^{-4}\sum_{i<j}\Big[\sum_k \mu_k^{-1/2}\{(\partial_{\mu,k}\Delta_\mu V)(z_p)\cdot(\partial_{\mu,k}B_{ij})(z_p)\} \\ &\quad -(\Delta_\mu B_{ij})(z_p)\Big]^2 \end{aligned}$$

(see Appendix). Therefore, if $D^{(2)}\neq 0$, $M^{(2)}$ has two simple eigenvalues $2E_{2,1}<2E_{2,2}$. Thus it suffices to apply Proposition 2.8 (iii).

In the particular case, where $V^{(3)}=0$ and $a^{(2)}=0$, we easily see that $H_1=0$ and hence we can apply Theorem 2.8 (ii). In this case, it is clear that

$$D^{(2)} = 2^{-4}\sum_{i<j}\big[(\Delta_\mu B_{ij})(z_p)\big]^2$$

and the eigenvalues $2E_{2,1}$ and $2E_{2,2}$ are given by

$$\begin{aligned} &(Q_2\phi_0,\phi_0)\mp 2^{-1}\sqrt{D^{(2)}} \\ &\quad = 2^{-3}\cdot 3\sum_{j=1}^{3}\mu_j + 2^{-4}\Big(\sum_{j=1}^{3}\sqrt{\mu_j}\Big)^2 + 2^{-4}\sum_{j=1}^{3}(\partial_{\mu,j}^4 V)(0) \\ &\qquad +2^{-3}\sum_{i<j}(\partial_{\mu,i}^2\partial_{\mu,j}^2 V)(0)\mp 2^{-3}\Big[\sum_{i<j}\{(\Delta_\mu B_{ij})(0)\}^2\Big]^{1/2}. \end{aligned} \tag{4.13}$$

Proof of (iii). Similarly as the proof of (ii), we apply Theorem 2.8 (iii) with $j_1=2, j_2=4$. Under the hypotheses of (iii), we can choose $E_1=E_3=0$ and we see that K_2 has a double eigenvalue $2E_2=2E_{2,i}$ as in (4.13) with $D^{(2)}=0$. Then the condition in the theorem is equivalent to $D^{(4)}\neq 0$. For precise calculation, see Appendix. Thus by the fact $D^{(4)}\neq 0$, $M^{(4)}$ has two simple eigenvalues $2E_{4,1}<2E_{4,2}$, where

$$\begin{aligned} 2E_{4,1} &= \frac{M_{11}^{(4)}+M_{22}^{(4)}-\sqrt{D^{(4)}}}{2}, \\ 2E_{4,2} &= \frac{M_{11}^{(4)}+M_{22}^{(4)}+\sqrt{D^{(4)}}}{2}. \end{aligned}$$

The result follows from the same arguments as (ii). This completes the proof of Theorem 4.1. □

In the case of single well, we obtain a corollary of Theorem 4.1.

Corollary 4.3. *Assume that the well U consists of a single point z. Then we have the following:*

(i) *If* $B(z) \neq 0$ *and* $|B(z)| < \sqrt{2}s_1$, $P_V^h(a)$ *has the first two non-degenerate eigenvalues* $\lambda_i(h)$ $(i = 1,2)$ *which satisfy that there exists a constant* $C > 0$ *such that for small* $h > 0$,

$$h|B(z)|/\sqrt{2} - C^{-1}h^{3/2} \leq \lambda_2(h) - \lambda_1(h) \leq h|B(z)|/\sqrt{2} + Ch^{3/2}.$$

(ii) *If* $B(z) = 0$ *and* $D^{(2)} \neq 0$, *then* $P_V^h(a)$ *has the first two non-degenerate eigenvalues* $\lambda_i(h)$ $(i = 1,2)$ *which satisfy that there exists a constant* $C > 0$ *such that for small* $h > 0$,

$$\frac{1}{2}\sqrt{D^{(2)}}h^2 - C^{-1}h^{5/2} \leq \lambda_2(h) - \lambda_1(h) \leq \frac{1}{2}\sqrt{D^{(2)}}h^2 + Ch^{5/2}.$$

(iii) *Assume that the hypotheses of Theorem* 4.1 *(iii) hold and that* $D^{(4)} \neq 0$, *then* $P_V^h(a)$ *has the first two non-degenerate eigenvalues* $\lambda_i(h)$ $(i = 1,2)$ *which satisfy that there exists a constant* $C > 0$ *such that for small* $h > 0$,

$$\frac{1}{2}\sqrt{D^{(4)}}h^3 - C^{-1}h^{7/2} \leq \lambda_2(h) - \lambda_1(h) \leq \frac{1}{2}\sqrt{D^{(4)}}h^3 + Ch^{7/2}.$$

This corollary is an improvement of [12].

5. An Example

In this section, we consider an example as an application of Theorem 4.1.

Let

$$\begin{aligned} a_1(x) &= a_{10}x_2 + a_{11}x_1^2x_2 + a_{12}x_1^4x_2, \\ a_2(x) &= a_{20}x_1 + a_{21}x_1x_2^2 + a_{22}x_1x_2^4, \\ a_3(x) &= 0, \end{aligned}$$

where a_{ij} are real constants and $V(x) = -e^{-|x|^2/2}$. Then it is clear that the operator

$$P_V^h(a) = \alpha \cdot D^h(a) + \alpha_4 + V(x)I_4 \quad \text{on } \mathcal{H} = L^2(\mathbf{R}^3; \mathbf{C}^4)$$

satisfies the hypotheses (S.1), (V.1), (V.2) and (V.3) with the well $U = U^- = \{0\}$ and $V''(0) = I_2$. Clearly it holds that

$$\begin{aligned} B_{21}(x) &= \partial_2 a_1(x) - \partial_1 a_2(x) = a_{10} - a_{20} + a_{11}x_1^2 - a_{21}x_2^2 \\ &\quad + a_{12}x_1^4 - a_{22}x_2^4, \\ B_{13}(x) &= B_{23}(x) = 0. \end{aligned}$$

Hence the operator H_0 defined as in Theorem 4.1 becomes

$$H_0 = \left[(i\partial_1 - Bx_2/2)^2 + (i\partial_2 + Bx_1/2)^2 - \partial_3^2 + |x|^2\right] I_2 - \sigma_3 B\,,$$

where $B = B_{12}(0) = a_{20} - a_{10}$. It follows from an elementary calculation that the eigenvalues $\pm is_j \quad (j = 1, 2, 3)$ of the 6×6-matrix

$$M = \begin{bmatrix} \widetilde{B} & I_3 \\ -I_3 & 0 \end{bmatrix}, \quad \text{where } \widetilde{B} = \begin{bmatrix} 0 & B & 0 \\ -B & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

are given by $s_1 = \frac{1}{2}\{\sqrt{4+B^2} - |B|\}, s_2 = 1, s_3 = \frac{1}{2}\{\sqrt{4+B^2} + |B|\}$. Thus we see that

$$\sigma(H_0) = \{\sum_{j=1}^{3}(2n_j + 1)s_j \pm |B|; n = (n_1, n_2, n_3) \in (\mathbf{Z}_+)^3\}.$$

When $a_{10} \neq a_{20}$, i.e., $B \neq 0$, the ground state energy of H_0 is equal to $2E_0 = \sum_{j=1}^{3} s_j - |B| = 1 + \sqrt{4 + |B|^2} - |B|$ and non-degenerate. Thus we see that $P_V^h(a)$ has a non-degenerate eigenvalue $\lambda_0(h)$ which satisfies

$$\lambda_0(h) = hE_0 + O(h^{3/2}) \quad \text{as } h \downarrow 0\,, \tag{5.1}$$

where $E_0 = \left\{1 + \sqrt{4 + |a_{10} - a_{20}|^2} - |a_{10} - a_{20}|\right\}/2$.

Note that if $|a_{10} - a_{20}| < 1/\sqrt{2}$, the second eigenvalue of H_0 is also non-degenerate and so we see that $P_V^h(a)$ has a non-degenerate eigenvalues $\lambda_1(h)$ which satisfies

$$\lambda_1(h) = hE_1 + O(h^{3/2}) \quad \text{as } h \downarrow 0\,, \tag{5.2}$$

where $E_1 = \left\{1 + \sqrt{4 + |a_{10} - a_{20}|^2} + |a_{10} - a_{20}|\right\}/2$. Moreover, in view of Corollary 4.3, there exists a constant $C > 0$ such that

$$|a_{10} - a_{20}|h - Ch^{3/2} \leq \lambda_1(h) - \lambda_0(h) \leq |a_{10} - a_{20}|h + Ch^{3/2}.$$

When $a_{10} = a_{20}$, i.e., $B_{12}(0) = 0$, we see that

$$H_0 = (-\Delta + |x|^2)I_2 \quad \text{on } L^2(\mathbf{R}^3; \mathbf{C}^2)$$

and that

$$\sigma(H_0) = \sigma_{\text{disc}}(H_0) = \{\mu_\alpha := \sum_{j=1}^{3}(2\alpha_j + 1); \alpha = (\alpha_1, \alpha_2, \alpha_3) \in (\mathbf{Z}_+)^3\}.$$

The ground state energy of H_0 is $2E_0 = 3$ which is double and the corresponding eigenspace becomes

$$\mathcal{H} = [\phi_0^+, \phi_0^-] := \left[\begin{bmatrix} \phi_0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ \phi_0 \end{bmatrix} \right],$$

where $\phi_0(x) = \phi_{(0,0,0)}(x) = \pi^{-3/4} e^{-|x|^2/2}$ is the ground state of the harmonic oscillator $H_{00} = -\Delta + |x|^2$ on $L^2(\mathbf{R}^3)$. Let $\phi_\alpha(x)$ be the orthonormalized eigenfunctions corresponding to the eigenvalues μ_α of H_{00}. We apply Theorem 4.1 (ii) with $\mu_j = 1$. Then, we get $D^{(2)} = \frac{1}{4}|a_{11} - a_{21}|^2$. Therefore if $a_{11} \neq a_{21}$, by (4.13) with $\mu_j = 1$, we see that $\Pi_{\mathcal{H}_0} H_2\big|_{\mathcal{H}_0}$ has two non-degenerate eigenvalues $b^\pm = \frac{3}{4} \pm \frac{1}{4}|a_{11} - a_{21}|$. As a result, if $a_{11} \neq a_{21}$, $P_V^h(a)$ has two non-degenerate eigenvalues $\lambda_0^\pm(h)$ such that

$$\lambda_0^\pm(h) = \frac{3}{2}h + \frac{1}{2}b^\pm h^2 + O(h^{5/2}) \quad \text{as } h \downarrow 0 . \tag{5.3}$$

Moreover, in view of Corollary 4.3, there exists a constant $C > 0$ such that

$$\frac{1}{4}|a_{11} - a_{21}|h^2 - Ch^{5/2} \leq \lambda_0^+(h) - \lambda_0^-(h) \leq \frac{1}{4}|a_{11} - a_{21}|h^2 + Ch^{5/2}.$$

We consider the case, where $a_{10} = a_{20}$, $a_{11} = a_{21}$ and $a_{12} \neq a_{22}$. In this case, we easily see that $H_1 = H_3 = 0$ and we can choose $2E_0 = 3, E_1 = 0, 2E_2 = 3/4$. We compute the components of the representation matrix $M^{(4)}$ of $K_4 = \Pi_{\mathcal{H}_0}\left[-H_2(H_0 - 2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_0} H_2 + H_4\right]\big|_{\mathcal{H}_0}$ with respect to ϕ_0^+, ϕ_0^-. Since $B_{23}(x) = B_{13}(x) \equiv 0$, we have $M_{12}^{(4)} = M_{21}^{(4)} = 0$. By (4.10), we can put $M_{11}^{(2l)} = -I_1 - I_2 + 2I_3 - I_4 + I_5 - I_6$, where

$$\begin{aligned}
I_1 &= \big((H_{00} - 2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}} A_{20}\phi_0, A_{20}\phi_0\big), \\
I_2 &= \big((H_{00} - 2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}} Q_2\phi_0, Q_2\phi_0\big), \\
I_3 &= \big(((H_{00} - 2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}} Q_2\phi_0, B_{12}^{(2)}\phi_0\big), \\
I_4 &= \big(((H_{00} - 2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}} B_{12}^{(2)}\phi_0, B_{12}^{(2)}\phi_0\big), \\
I_5 &= (Q_4\phi_0, \phi_0), \\
I_6 &= (B_{12}^{(4)}\phi_0, \phi_0).
\end{aligned}$$

Since $A_{20} = 2i(2a_{11}x_1x_2 + a_{11}x_1^2x_2\partial_1 + a_{11}x_1x_2^2\partial_2)$ and $\partial_i\phi_0 = -x_i\phi_0$, using (A.1) and (A.2) in Appendix, we have

$$A_{20}\phi_0 = -ia_{11}\phi_{(1,1,0)} - ia_{11}2^{-1/2} \cdot 3^{1/2}(\phi_{(3,1,0)} + \phi_{(1,3,0)}).$$

Since $(H_{00}-2E_0)^{-1}\phi_\alpha = (2|\alpha|)^{-1}\phi_\alpha$ for $\alpha \neq 0$, we have

$$\begin{aligned}&(H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}} A_{20}\phi_0\\ &= -i2^{-2}a_{11}\phi_{(1,1,0)} - i2^{-7/2}\cdot 3^{1/2}a_{11}(\phi_{(3,1,0)}+\phi_{(1,3,0)}).\end{aligned}$$

Thus we have $I_1 = -2^{-3}\cdot 5a_{11}^2$. Similar computations lead to

$$\begin{aligned}Q_2\phi_0 &= -2^{-3/2}\cdot 3(\phi_{(2,0,0)}+\phi_{(0,2,0)}+\phi_{(0,0,2)})\\ &\quad +2^{-2}\cdot 3\phi_0,\\ (H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}}Q_2\phi_0 &= -2^{-7/2}\cdot 3(\phi_{(2,0,0)}+\phi_{(0,2,0)}+\phi_{(0,0,2)}),\\ B_{12}^{(2)}\phi_0 &= 2^{-1/2}a_{11}(\phi_{(0,2,0)}-\phi_{(2,0,0)}),\\ \Pi_{\mathcal{H}_{00}}Q_4\phi_0 &= (2^{-2}\cdot 3a_{11}^2 + 2^{-5}\cdot 13)\phi_0,\\ \Pi_{\mathcal{H}_{00}}B_{12}^{(4)}\phi_0 &= 2^{-2}\cdot 3(a_{22}-a_{12})\phi_0.\end{aligned}$$

Thus we have $I_2 = 2^{-5}\cdot 3^3$, $I_3 = 0$, $I_4 = 2^{-2}a_{11}^2$, $I_5 = 2^{-2}\cdot 3a_{11}^2 + 2^{-5}\cdot 13$, $I_6 = 2^{-2}\cdot 3(a_{22}-a_{12})$. Therefore, if $M_{11}^{(4)} \neq M_{22}^{(4)}$, i.e., $a_{22}\neq a_{12}$, $M^{(4)}$ has two simple eigenvalues $c^{\pm} = 2^{-3}\cdot 3^2 a_{11}^2 + 2^{-3}\cdot 5 \pm 2^{-2}\cdot 3|a_{22}-a_{12}|$.

As a result, $P_V^h(a)$ has the first two simple eigenvalues $\lambda_0^{\pm}(h)$ such that

$$\lambda_0^{\pm}(h) = \frac{3}{2}h + \frac{3}{8}h^2 + \frac{1}{2}c^{\pm}h^3 + O(h^{7/2}) \quad \text{as } h\downarrow 0. \tag{5.4}$$

Moreover, in view of Corollary 4.3, there exists a constant $C>0$ such that

$$\begin{aligned}2^{-2}\cdot 3|a_{12}-a_{22}|h^3 - Ch^{7/2} &\leq \lambda_0^+(h)-\lambda_0^-(h)\\ &\leq 2^{-2}\cdot 3|a_{12}-a_{22}|h^3 + Ch^{7/2}.\end{aligned}$$

When $a_{10}=a_{20}$, $a_{11}=a_{21}$ and $a_{12}=a_{22}$, we see that for every $l\geq 0$, H_l is symmetric with respect to the exchange of x_1 and x_2 variables and so is H^h. Define an operator J on $L^2(\mathbf{R}^3;\mathbf{C}^2)$ so that

$$J\begin{bmatrix} u_+(x_1,x_2,x_3)\\ u_-(x_1,x_2,x_3)\end{bmatrix} = \sigma_2\begin{bmatrix}\overline{u_+}(x_2,x_1,x_3)\\ \overline{u_-}(x_2,x_1,x_3)\end{bmatrix}.$$

Then all the hypotheses of Theorem 2.9 hold. Since $\dim\mathcal{H}_0 = 2$, it follows from Theorem 2.9 that $P_V^h(a)$ has a double eigenvalue $\lambda_0(h)$ which satisfies that

$$\lambda_0(h) = \frac{3}{2}h + O(h^{3/2}) \quad \text{as } h\downarrow 0. \tag{5.5}$$

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Appendix

In this appendix, we examine the concrete values of the discriminant $D^{(2l)}$ of the characteristic equation of $M^{(2l)}$ for $l = 1, 2$ which are appeared in Theorem 4.1.

It is well-known that the harmonic oscillator $P = -d^2/dt^2 + t^2$ on $L^2(\mathbf{R})$ has the eigenvalues $\lambda_j = 2j + 1 \quad (j \in \mathbf{Z}_+)$ with the corresponding orthonormal eigenfunctions $\psi_j(t)$:

$$\psi_j(t) = \frac{1}{\sqrt{j!}2^{j/2}}\left(-\frac{d}{dt} + t\right)^j \psi_0(t) = \frac{1}{\sqrt{j!}2^{j/2}\pi^{1/4}} H_j(t)e^{-t^2/2},$$

$\psi_0(t) = \pi^{-1/4}e^{-t^2/2}$, where $H_j(t)$ is j-th Hermite polynomial and so satisfies an equation

$$\psi_{j+1}(t) - \frac{\sqrt{2}}{\sqrt{j+1}}t\psi_j(t) + \frac{\sqrt{j}}{\sqrt{j+1}}\psi_{j-1}(t) = 0 \quad (j = 1, 2, \ldots).$$

Using this formula, we see that $t^j\psi_0$ is a linear combination of ϕ_{j-2l} $(0 \le l \le [j/2])$, where $[a]$ denotes the maximal integer equal to or less than a.

For the operator $-d^2/dt^2 + \mu t^2 \quad (\mu > 0)$, we can see that the eigenvalues are $\mu^{1/2}\lambda_j \quad (j \in \mathbf{Z}_+)$ and the corresponding orthonormal eigenfunctions become $\phi_j(t) = \mu^{1/8}\psi_j(\mu^{1/4}t)$. Since we need the concrete representations of $t^j\phi_0$ for $0 \le j \le 6$, we write

$$t^j\phi_0 = \mu^{-j/4}\sum_{l=0}^{[j/2]} c^j_{j-2l}\phi_{j-2l} \tag{A.1}$$

and list c^j_{j-2l}, as follows:

$$\begin{aligned}
&c^1_1 = 2^{-1/2},\\
&c^2_2 = 2^{-1/2}, \quad c^2_0 = 2^{-1},\\
&c^3_3 = 2^{-1}\cdot 3^{1/2}, \quad c^3_1 = 2^{-3/2}\cdot 3,\\
&c^4_4 = 2^{-1/2}\cdot 3^{1/2}, \quad c^4_2 = 2^{-1/2}\cdot 3, \quad c^4_0 = 2^{-2}\cdot 3,\\
&c^5_5 = 2^{-1}\cdot 3^{1/2}\cdot 5^{1/2}, \quad c^5_3 = 2^{-1}\cdot 3^{1/2}\cdot 5, \quad c^5_1 = 2^{-5/2}\cdot 3\cdot 5,\\
&c^6_6 = 2^{-1}\cdot 3\cdot 5^{1/2}, \quad c^6_4 = 2^{-3/2}\cdot 3^{3/2}\cdot 5,\\
&c^6_2 = 2^{-5/2}\cdot 3^2\cdot 5, \quad c^6_0 = 2^{-3}\cdot 3\cdot 5.
\end{aligned} \tag{A.2}$$

Now $P_\mu = -\Delta + \sum_{j=1}^3 \mu_j x_j^2 \quad (\mu_j > 0)$ on $L^2(\mathbf{R}^3)$ has the eigenvalues $\mu_\alpha = \sum_{j=1}^3 \sqrt{\mu_j}(2\alpha_j + 1)$ for $\alpha = (\alpha_1, \alpha_2, \alpha_3) \in (\mathbf{Z}_+)^3$ and the associated orthonormal eigenfunctions can be written by $\phi_\alpha(x) = \phi_{\alpha_1}(x_1)\phi_{\alpha_2}(x_2)\phi_{\alpha_3}(x_3)$. In particular,

$$\phi_0(x) = \phi_{(0,0,0)}(x) = (\mu_1\mu_2\mu_3)^{1/8}\pi^{-3/4}\exp(-\sum_{j=1}^3 \sqrt{\mu_j}x_j^2).$$

We need to calculate $D^{(2l)}$ for $l = 1$ or $l = 2$ in (4.11). By (A.1), we get the following formula

$$x^\alpha \phi_0(x) = \mu^{-\alpha/4} \sum_{\beta \le [\alpha/2]} c^\alpha_{\alpha-2\beta}\phi_{\alpha-2\beta}(x). \tag{A.3}$$

Here we used the notations

$$\begin{aligned} \mu^{-\alpha/4} &= \mu_1^{-\alpha_1/4}\mu_2^{-\alpha_2/4}\mu_3^{-\alpha_3/4}, \\ c^\alpha_{\alpha-2\beta} &= c^{\alpha_1}_{\alpha_1-2\beta_1}c^{\alpha_2}_{\alpha_2-2\beta_2}c^{\alpha_3}_{\alpha_3-2\beta_3}, \end{aligned}$$

and $\beta \le [\alpha/2]$ means $\beta_j \le [\alpha_j/2]$ for $j = 1, 2, 3$.

For $l = 1$, by (4.3), we have

$$\overline{\Pi}_{\mathcal{H}_{00}} Q_1 \phi_0 = 2 \sum_{|\alpha|=3} \frac{(\partial_\mu^\alpha V)(0)}{\alpha!} \sum_{\beta \le [\alpha/2]} c^\alpha_{\alpha-2\beta}\phi_{\alpha-2\beta}.$$

Therefore, it follows that

$$\begin{aligned} &(H_{00} - 2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}} Q_1 \phi_0 \\ &\quad = \sum_{|\alpha|=3} \frac{(\partial_\mu^\alpha V)(0)}{\alpha!} \sum_{\beta \le [\alpha/2]} c^\alpha_{\alpha-2\beta}(\sqrt{\mu}\cdot(\alpha-2\beta))^{-1}\phi_{\alpha-2\beta}\,, \end{aligned}$$

where $\sqrt{\mu}\cdot(\alpha - 2\beta) = \sum_{j=1}^3 \sqrt{\mu_j}(\alpha_j - 2\beta_j)$. Since

$$B^{(1)}_{ij}\phi_0 = c^1_1 \sum_{|\gamma|=1} (\partial_\mu^\gamma B_{ij})(0)\phi_\gamma,$$

the orthonormality of ϕ_α leads to

$$\begin{aligned} &2\big((H_{00} - 2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}} Q_1\phi_0, B^{(1)}_{ij}\phi_0\big) \\ &\quad = 2\sum_{|\alpha|=3} \frac{(\partial_\mu^\alpha V)(0)}{\alpha!} \sum_{\beta \le [\alpha/2], \alpha \ne 2\beta} c^\alpha_{\alpha-2\beta} c^1_1 \sum_{|\gamma|=1} (\partial_\mu^\gamma B_{ij})(0) \\ &\qquad \times (\sqrt{\mu}\cdot(\alpha - 2\beta))^{-1}\delta_{\alpha-2\beta,\gamma}. \end{aligned}$$

For example, for $\gamma = (1,0,0)$, the Kronecker delta $\delta_{\alpha-2\beta,\gamma}$ survives only for $\alpha = (3,0,0),(1,2,0),(1,0,2)$ with $\beta = (1,0,0)$, $(0,1,0)$, $(0,0,1)$, respectively. Thus we have

$$\begin{aligned}&2\big((H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}}Q_1\phi_0, B_{ij}^{(1)}\phi_0\big)\\&= 2^{-2}\sum_{k=1}^{3}\mu_k^{-1/2}(\partial_{\mu,k}\Delta_\mu V)(0)\cdot(\partial_{\mu,k}B_{ij})(0).\end{aligned}$$

Since

$$(B_{ij}^{(2)}\phi_0,\phi_0) = \sum_{|\alpha|=2}\frac{(\partial^\alpha B_{ij})(0)}{\alpha!}(x^\alpha\phi_0,\phi_0) = 2^{-2}(\Delta_\mu B_{ij})(0),$$

it is easy to see that the left hand side of (4.6) is equal to $2^{-2}D^{(2)}$.

For $l=2$, we need to calculate $D^{(4)} = 2^2\sum_{i<j}(2E_{ij}^{(1)} - E_{ij}^{(2)})^2$, where

$$\begin{aligned}E_{ij}^{(1)} &= \big(Q_2\phi_0, (H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}}B_{ij}^{(2)}\phi_0\big),\\ E_{ij}^{(2)} &= (B_{ij}^{(4)}\phi_0,\phi_0).\end{aligned}$$

Since ϕ_0 is an even function with respect to x_1, x_2, x_3, it follows from (A.2) and (A.3) that

$$\begin{aligned}E_{ij}^{(2)} &= \sum_{|\alpha|=4}\frac{(\partial^\alpha B_{ij})(0)}{\alpha!}(x^\alpha\phi_0,\phi_0)\\ &= \sum_{k=1}^{3}\frac{(\partial_k^4 B_{ij})(0)}{4!}(x_k^4\phi_0,\phi_0) + \sum_{k<l}\frac{(\partial_k^2\partial_l^2 B_{ij})(0)}{2!\cdot 2!}(x_k^2x_l^2\phi_0,\phi_0)\\ &= 2^{-5}(\Delta_\mu^2 B_{ij})(0).\end{aligned}$$

We calculate $E_{ij}^{(1)}$. Using (A.2) and (A.3), we have

$$\begin{aligned}\overline{\Pi}_{\mathcal{H}_{00}}B_{ij}^{(2)}\phi_0 &= \sum_{|\alpha|=2}\frac{(\partial^\alpha B_{ij})(0)}{\alpha!}\overline{\Pi}_{\mathcal{H}_{00}}x^\alpha\phi_0\\ &= \sum_{|\alpha|=2}\frac{(\partial^\alpha B_{ij})(0)}{\alpha!}\sum_{\beta\le[\alpha/2],\alpha\ne 2\beta}c_{\alpha-2\beta}^{\alpha}\phi_{\alpha-2\beta}.\end{aligned}$$

Therefore, we have

$$(H_{00}-2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}}B_{ij}^{(2)}\phi_0 = \sum_{|\alpha|=2}\frac{(\partial^\alpha B_{ij})(0)}{\alpha!}(2\sqrt{\mu}\cdot\alpha)^{-1}\phi_\alpha.$$

Let $\mathcal{K}$ be the subspace spanned by ϕ_α for $|\alpha| = 2$. In order to compute $E_{ij}^{(1)}$, it suffices to find

$$\Pi_{\mathcal{K}} Q_2 \phi_0 = 2\Pi_{\mathcal{K}} V^{(4)}\phi_0 + \Pi_{\mathcal{K}}(V^{(2)})^2\phi_0 - (\sum_{j=1}^{3} \sqrt{\mu_j})\Pi_{\mathcal{K}} V^{(2)}\phi_0.$$

Since $V^{(2)} = \sum_{j=1}^3 \mu_j x_j^2/2$, we easily see that

$$\begin{aligned} &\Pi_{\mathcal{K}}(V^{(2)})^2\phi_0 - (\sum_{j=1}^{3} \sqrt{\mu_j})\Pi_{\mathcal{K}} V^{(2)}\phi_0 \\ &= 2^{-5/2}\big[\mu_1^{1/2}(\mu_1^{1/2} - \mu_2^{1/2} - \mu_3^{1/2})\phi_{(2,0,0)} \\ &\quad +\mu_2^{1/2}(\mu_2^{1/2} - \mu_1^{1/2} - \mu_3^{1/2})\phi_{(0,2,0)} \\ &\quad +\mu_3^{1/2}(\mu_3^{1/2} - \mu_1^{1/2} - \mu_2^{1/2})\phi_{(0,0,2)}\big]. \end{aligned}$$

Therefore, we obtain

$$\begin{aligned} &\big((\Pi_{\mathcal{K}}(V^{(2)})^2 - (\sum_{j=1}^{3} \sqrt{\mu_j})\Pi_{\mathcal{K}} V^{(2)})\phi_0, (H_{00} - 2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}} B_{ij}^{(2)}\phi_0\big) \\ &\qquad = 2^{-6}\big[\sum_{k=1}^{3} \mu_k^{1/2}(\partial_{\mu,k}^2 B_{ij})(0) - \sum_{k\neq l} \mu_k^{1/2}(\partial_{\mu,l}^2 B_{ij})(0)\big]. \end{aligned}$$

Finally, we calculate $\widetilde{E}_{ij}^{(2)} := 2((H_{00} - 2E_0)^{-1}\overline{\Pi}_{\mathcal{H}_{00}} V^{(4)}\phi_0, B_{ij}^{(2)}\phi_0)$. Using (A.3) and the orthonormality of ϕ_α, we see that

$$\begin{aligned} \widetilde{E}_{ij}^{(2)} \quad &= \quad \sum_{|\gamma|=2}\sum_{|\alpha|=4}\sum_{\beta\leq[\alpha/2],|\alpha-2\beta|=2} \frac{\partial_\mu^\alpha V(0)}{\alpha!}\frac{\partial_\mu^\gamma B_{ij}(0)}{\gamma!} \\ &\quad \times(\sqrt{\mu}\cdot\gamma)^{-1} C_{\alpha-2\beta}^{\alpha} c_\gamma^\gamma \delta_{\alpha-2\beta,\gamma}. \end{aligned}$$

If we use (A.1), an elementary calculation leads to

$$\widetilde{E}_{ij}^{(2)} = 2^{-5}\sum_{k,l=1}^{3} (\sqrt{\mu_k} + \sqrt{\mu_l})^{-1}(\partial_{\mu,k}\partial_{\mu,k}\Delta_\mu V)(0)\cdot(\partial_{\mu,k}\partial_{\mu,l} B_{ij})(0).$$

Thus we see that

$$D^{(4)} = 2^{-6} \sum_{i<j} \Big[\sum_{k,l=1}^{3} (\sqrt{\mu_k} + \sqrt{\mu_l})^{-1} (\partial_{\mu,k}\partial_{\mu,l}\Delta_\mu V)(0) \cdot (\partial_{\mu,k}\partial_{\mu,l} B_{ij})(0) + \sum_{k=1}^{3} \mu_k^{1/2} (\partial_{\mu,k}^2 B_{ij})(0) - \sum_{k \neq l} \mu_k^{1/2} (\partial_{\mu,l}^2 B_{ij})(0) - (\Delta_\mu^2 B_{ij})(0) \Big]^2.$$