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Tunnelling instability via perturbation theory

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Abstract. We study the semiclassical limit of low lying states in a multiwell potential by rigorous perturbative techniques. In particular we obtain in a simple way tunnelling instability and localisation of wavefunctions under small deformations of symmetric potentials.

1. Introduction

Problems of resonant states have acquired a considerable importance in the recent literature in mathematical physics. There are both mathematical and physical reasons for this trend. From the mathematical point of view the study of resonant states or tunnelling leads to a singular perturbation problem as it requires the solution of the Schrödinger equation for small values of the coefficients multiplying the kinetic energy, i.e. the highest derivative in the equation. Physicists call it the semiclassical limit. Only very recently were sufficiently powerful techniques developed to deal satisfactorily with such a problem (see e.g. Helffer and Siöstrand 1983). From the physical standpoint, understanding tunnelling appears as a central issue in the study of quantum disordered systems, in particular in the description of the metal–insulator transition. The control of tunnelling is a key point in the recent analysis by Fröhlich and Spencer (1983) of the Anderson model for such a transition. Also molecular physics seems to require a deep understanding of the semiclassical limit to solve some of its basic issues, e.g. the compatibility of the traditional concept of molecule, as used by chemists, with quantum mechanics (Claverie and Diner 1980). Strangely enough, after almost sixty years of quantum mechanics this question is still considerably obscure. Localisation of wavefunctions seems to play an important role here too. Let us mention in passing a growing branch of solid state physics which presumably will need a serious theoretical command on tunnelling problems in the near future: the physics of superlattices (for an informal exposition see Dölher (1983)).

The tunnelling situations considered for a long time in the physics literature were characterised by the existence of symmetries. Typical is the treatment of the double well in the book of Landau and Lifshitz or the solution of simple problems exhibiting band structure in solid state physics. All this is reflected also in the first rigorous papers devoted to the problem which consider only symmetric potentials (Harrell 1978, 1980). As far as non-symmetric situations are concerned it has long been known that

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if in a symmetric double well the curvature of one of the minima is changed, tunnelling disappears and the wavefunction is completely localised in the minimum of smaller curvature. This case can be easily understood by simple min–max arguments.

What is much more difficult is to control what happens when symmetry breaking takes place far from the minima or on a small scale compared with the extension of the region over which tunnelling is effective in the symmetric non-perturbed situation. The latter case typically arises when we consider the effect of an impurity in a perfectly periodic and symmetric structure. The first investigations of non-symmetric situations led to the surprising conclusion that tunnelling is very sensitive to perturbations of the kinds described above. In fact it was proved in Jona-Lasinio *et al* (1981a, b) that localised perturbations far from the minima are sufficient to produce exponential localisation of the wavefunctions and variations of the level splittings which are exponentially large if compared with the symmetric splitting.

In other words tunnelling in stationary states is a highly unstable phenomenon. The mathematical techniques by which these results were obtained are somewhat exotic: they rely on probabilistic ideas which are not part of the usual way of thinking of the theoretical physicist.

In the present paper we rigorously show that perturbation theory is sufficient to understand the main features of tunnelling instability. It may be useful to compare briefly the two approaches. The techniques used in Jona-Lasinio *et al* (1981a, b) permit a very detailed analysis of the problem which is not based on a previous knowledge of the symmetric case. Actually they constitute a self-contained approach to the semiclassical limit in a wide spectrum of situations. They are in principle applicable in any dimension although in dimension greater than one they may not be so viable. The perturbation approach proposed here requires a previous knowledge of the symmetric case and can deal only with perturbations which are small on a scale depending on $\hbar$. However, the latter is not a real limitation because we are in fact interested in knowing which are the *smallest* perturbations which can destabilise tunnelling. Furthermore, besides its conceptual simplicity, perturbation theory does not present additional conceptual difficulties when the space dimension is greater than one.

In the present paper our considerations are limited to one-dimensional examples (for concreteness one may think of long molecules) but it is quite clear, especially in view of the results of Simon (1984a, b) which extend the one-dimensional eigenfunction estimates of Harrell (1978, 1980) to any arbitrary finite dimension, that dimensionality does not play any essential role.

The basic content of the paper is the following. We consider a potential periodic over a finite segment, locally perturbed by a C^∞ potential as indicated in figure 1.

The perturbation ΔV may be negative (full curve) or positive (dotted curve). The lowest band of the symmetric unperturbed potential is given by a set of N levels (N is the number of minima) exponentially close to each other and to the ground state. The exponential order of magnitude of the splitting is $e^{-2A/\hbar}$, $A=\int_0^\pi V(x)^{1/2}\,dx$. The corresponding eigenfunctions are equally distributed over the different minima.

We take the perturbation ΔV smaller than the distance between the lowest band and the next one, i.e. $\Delta V<o(\hbar)$, for example $\Delta V=o(\hbar^2)$. We then show that as far as the lowest band is concerned we can approximately diagonalise the perturbed Hamiltonian $H_{\text{sym}}+\Delta V$ on the localised Wannier functions associated to the lowest N eigenstates. The largest matrix elements involved are typically of the order $e^{-2B/\hbar}$, $B=\int_{a_2}^\pi V(x)^{1/2}\,dx$, which is also the order of magnitude of the largest splitting involved.

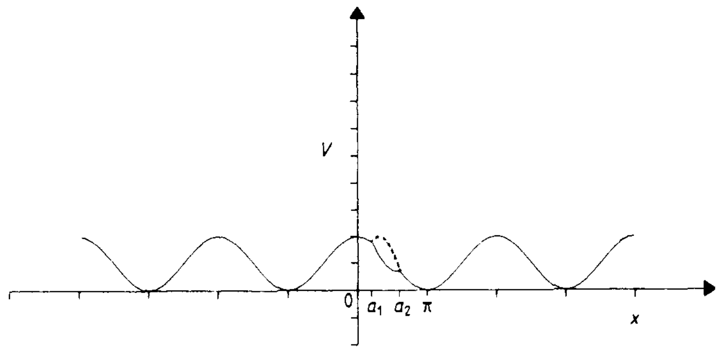

Figure 1.

Besides the exponential change in the splitting magnitude we find that the ratio between the value of the perturbed ground state wavefunction in the perturbed well and the value in any other one is of order $e^{(A-B)/\hbar}$ if $\Delta V < 0$. The same conclusion holds for the highest state of the band if $\Delta V > 0$.

We would like to conclude this introduction with a general comment. The development of techniques capable of dealing with non-symmetric tunnelling situations seems especially important as the functional integration techniques based on the instanton idea so popular in contemporary physics (Coleman 1977) have so far proved ineffective in approaching such problems.

The reason seems to be that a control is needed of the functional integral over an infinite time and the $T \to \infty$ limit cannot be interchanged with the $\hbar \to 0$ limit. In other words stationary action techniques work well in finite time intervals and extend to infinite time only under special symmetry conditions.

2. Perturbation of a symmetric multiwell potential

We consider in this section a potential $x \to V(x)$ periodic over the finite interval $(-2N\pi, 2N\pi)$, N positive integer, having $2N$ quadratic minima at $x = \pm x_k$, $x_k = (2k-1)\pi$, $k = 1, \ldots, N$. We assume furthermore $V(\pm x_k) = 0$, and we take for convenience $N = 2^p$, $p = 0, 1 \ldots$.

Specifically, the function $x \to V(x)$ can be constructed as follows: let $x \to F(x) \in C^\infty [-\pi, \pi]$, $F(x) \geq 0$, $F(x) = F(-x)$, $\lim_{x\to 0} F(x)x^{-2} = \omega^2 > 0$, $F'(x) = 0$ iff $x = 0$, $x = \pm\pi$. Then $x \to V(x)$ is defined by

(1) $V(x) = F(x - x_k)$, $2(k-1)\pi \leq x \leq 2k\pi$, $1 \leq k \leq N$,

(2) $V(x) = V(-x)$.

We denote by H_0 the Schrödinger operator $\hbar^2 p^2 + V(x)$, acting in $L^2(-2N\pi, 2N\pi)$ defined on $D(p^2)$ with periodic boundary conditions at $x = \pm 2N\pi$. Its well known relevant properties are collected in the following statement whose proof is briefly recalled in the appendix.

Proposition 2.1. Let $H_0 = H_0(\hbar)$ be as above. Then:

(1) $H_0(h)$ is self-adjoint and strictly positive.

(2) $H_0(h)$ has discrete spectrum, consisting of countably many simple eigenvalues $0 < \mu_1(\hbar) < \mu_2(\hbar) \ldots \uparrow +\infty$. For $\hbar$ suitably small, there are $C_i' > 0$, $C_i'' > 0$ such that

$$C_i'\hbar < \mu_i(\hbar) < C_i''\hbar, \qquad i = 1, 2, \ldots.$$

(3) Consider the set $B(\hbar)=\{\mu_i(\hbar): i=1,\ldots,2N\}$ hereafter referred to as 'the band'. Then there is $\varepsilon_i(\hbar)\downarrow 0$ as $\hbar\to 0$ such that the splittings $\Delta\mu_{ik}(\hbar)=\mu_i(\hbar)-\mu_k(\hbar)$, $i, k=1,\ldots,2N$, fulfil the estimate

$$\exp[-(2A+\varepsilon_1)/\hbar]<|\Delta\mu_{ik}(\hbar)|<\exp[-(2A-\varepsilon_1)/\hbar], \tag{2.1}$$

$$A=\int_0^\pi V(x)^{1/2}\,\mathrm{d}x. \tag{2.2}$$

Furthermore, the isolation distance of the band from the rest of the spectrum of $H_0(\hbar)$: $d(\hbar)=\min_{0<i\leq 2N<j}|\mu_i(\hbar)-\mu_j(\hbar)|$ is bounded below, $d(\hbar)>C\hbar$, for some $C>0$, $\hbar$ suitably small.

(4) Let $\psi_i(x,\hbar)$, $i=1,\ldots,2N$, be the band eigenfunctions. Then $\psi_i(x,\hbar)\in C^\infty(\mathbb{R})$ and for $\hbar$ suitably small $|\psi_i(x,\hbar)|$ has approximately equal maxima at $x=\pm x_k$, $k=1,\ldots,N$, i.e. there is $\eta=\eta(\hbar)\downarrow 0$ as $\hbar\to 0$ such that, if $\|\psi_i\|=1$, $i=1,\ldots,2N$:

$$1-\eta<|\psi_i(\pm x_{k_1},\hbar)/\psi_j(\pm x_{k_2},\hbar)|<1+\eta, \qquad k_1,k_2=1,\ldots,N;\ i,j=1,\ldots,2N.$$

(5) There is a unitary $2N\times 2N$ matrix $U=(c_{in})_{i,n=1\ldots 2N}$, $|c_{in}|=(2N)^{-1/2}$, such that the function $f_i(x,\hbar)=\Sigma_{k=1}^{2N} c_{ik}\psi_k\psi_k(x,\hbar)$ is concentrated (for $\hbar$ suitably small) near the ith minimum $\bar{x}_i=x_i$, $i=1,\ldots,N$; $\bar{x}_i=-x_{i-N}$, $i=N+1,\ldots,2N$. By this we mean that there are $0<\alpha<\frac{1}{2}$, $0<q(\hbar)<\hbar^\alpha$, such that, for $\pi>y_i=x-\bar{x}_i>q(\hbar)$ (and analogously for $-\pi<y_i<-q(\hbar)$) and some $\varepsilon(\hbar)\downarrow 0$ as $\hbar\downarrow 0$,

$$\exp[-(A+\varepsilon)/\hbar]\exp\left(\int_{y_i}^{\pi} V(t)^{1/2}\,\mathrm{d}t/\hbar\right)$$
$$<|f_i(x,\hbar)|<\exp[-(A-\varepsilon)/\hbar]\exp\left(\int_{y_i}^{\pi} V(t)^{1/2}\,\mathrm{d}t/\hbar\right) \qquad i=1,\ldots,2N, \tag{2.3}$$

while for $|y_i|\geq\pi$

$$|f_i(x,\hbar)|<\exp[-(A-\varepsilon)/\hbar]. \tag{2.4}$$

Let us now introduce a localised perturbation in the first well (it is of course irrelevant to consider it in any other well). Let therefore $x\to\Delta V(x)$ be in $C_0^\infty((0,2\pi)\backslash(\pi-q(\hbar),\pi+q(\hbar))$. For definitness we take supp $\Delta V=(a_1,a_2)$, $0<a_1<a_2<\pi-q(\hbar)$, and ΔV of constant sign, $\Delta V>0$ or $\Delta V<0$, $x\in(a_1,a_2)$. Then we have the following obvious estimate.

Lemma 2.2. Let $\Delta V_{ik}=\langle f_i,\Delta V f_k\rangle$, and $\varepsilon=\varepsilon(\hbar)$ be as above. Then for any η small enough, $a_2-a_1>\eta_1>0$, there is $\eta=\eta(\hbar)\to 0$ as $\hbar\downarrow 0$ such that

$$\exp[-2(B_1+\eta)/\hbar]<|\Delta V_{11}|<\exp[-2(B-\eta)/\hbar], \tag{2.5}$$

$$|\Delta V_{ik}|<\exp[-(A+B-2\eta)/\hbar], \qquad 1\neq i\neq k;$$

$$|\Delta V_{ii}|<\exp[-2(A-\eta)/\hbar], \qquad i\neq 1, \tag{2.6}$$

where

$$B=\int_{a_2}^{\pi} V(x)^{1/2}\,\mathrm{d}x, \qquad B_1=\int_{a_2-\eta_1}^{\pi} V(x)^{1/2}\,\mathrm{d}x.$$

Proof. We compute $\Delta V_{ij} = \int_{a_1}^{a_2} \Delta V(x) f_i(x) \bar{f}_j(x)\,\mathrm{d}x$. By (2.3):

$$\exp[-2(A+\varepsilon)/\hbar] \int_{a_1}^{a_2} |\Delta V(x)| \exp\left(2\int_0^x V(t)^{1/2}\,\mathrm{d}t/\hbar\right)\mathrm{d}x$$
$$< |\Delta V_{11}| < \exp[-2(A-\varepsilon)/\hbar] \int_{a_1}^{a_2} |\Delta V(x)| \exp\left(2\int_0^x V(t)^{1/2}\,\mathrm{d}t/\hbar\right)\mathrm{d}x \tag{2.7}$$

whence

$$\exp\left[-2\left(A - \int_0^{a_2-\eta_1} V(t)^{1/2}\,\mathrm{d}t + \varepsilon\right)\Big/\hbar\right] \int_{a_2-\eta_1}^{a_2} |\Delta V(x)|\,\mathrm{d}x < |\Delta V_{11}|$$
$$< \exp\left[-2\left(A - \int_0^{a_2} V(t)^{1/2}\,\mathrm{d}t - \varepsilon\right)\right] \int_{a_1}^{a_2} |\Delta V(x)\,\mathrm{d}x.$$

Taking $\eta = \varepsilon - \frac{1}{2}\hbar \ln \int_{a_2-\eta_1}^{a_2} |\Delta V(x)|\,\mathrm{d}x$ we get (2.5). On the other hand $|\Delta V_{ik}| \leqslant \int_{a_1}^{a_2} |\Delta V(x)|\,|f_1(x)|\,|\bar{f}_j(x)|\,\mathrm{d}x$ whence (2.6) by (2.4).

Denote now by H the Schrödinger operator $H_0 + \Delta V$, defined on $D(H_0)$. Since the multiplication by ΔV is bounded as an operator in $L^2(\mathbb{R})$, it is bounded also with respect to H_0 with relative bound zero. Hence (see e.g. Reed and Simon (1975–8), theorems X.12, XII.8, XIII.14) H is self-adjoint, bounded below, has discrete spectrum and the eigenvalues of H_0 are stable with respect to the perturbation ΔV (the technical definition is recalled below). The strength of the perturbation is measured by $\|\Delta V\|_\infty = \max_{a_1 \leqslant x \leqslant a_2} |\Delta V(x)| \equiv b$. The most interesting case is clearly b arbitrarily small: accordingly we take b of order d^2, where $d = \mathrm{O}(\hbar)$ is the isolation distance of $B(\hbar)$ from $\sigma(H_0) \backslash B(\hbar)$.

We can now state our first result, i.e. the exponential instability of the eigenvalue splitting.

Proposition 2.3. There is $\delta > 0$ such that, for all $0 < \hbar < \delta$:

(1) The operator H has exactly $2N$ eigenvalues $E_i(\hbar)$, $i = 1, \ldots, 2N$, such that $|E_i(\hbar) - \mu_j(\hbar)| \leqslant C_{ij} b$, $i, j = 1, \ldots, 2N$, for some $C_{i,j} > 0$ independent of $\hbar$.

(2) Let $E_1(\hbar) = \max_{1 \leqslant i \leqslant 2N} E_i(\hbar)$ for $\Delta V > 0$, $E_1(\hbar) = \min_{1 \leqslant i \leqslant 2N} E_i(\hbar)$ for $\Delta V < 0$, and let $\Delta E_{i,k} = E_i(\hbar) - E_k(\hbar)$, $i \neq k = 1, \ldots, 2N$. Then for $b < \frac{1}{2}d$, B and B_1 as above, there is $\varepsilon_2(\hbar) \downarrow 0$ as $\hbar \downarrow 0$ such that

$$\exp[-2(B_1+\varepsilon)/\hbar] < |\Delta E_{1,k}| < \exp[-2(B-\varepsilon)/\hbar]. \tag{2.8}$$

Remark. This is exactly the result of Jona-Lasinio *et al* (1981a, b). It shows the exponential instability of the tunnelling because $A > B_1 \geqslant B$, and $\varepsilon_2(\hbar) \downarrow 0$ as $\hbar \downarrow 0$. Let us first prove the following auxiliary statement.

Lemma 2.4. Let Γ be the circle $\{z \in \mathbb{C}: |z - \mu_1(\hbar)| = \frac{1}{2}d\}$. Let $R(z, H_0) = (H_0 - z)^{-1}$, $z \notin \sigma(H_0)$, be the resolvent of H_0, and let, for $z \in \Gamma$,

$$\begin{aligned} Q_1(z) &= -(\Delta V R(z, H_0))^2 (1 + \Delta V R(z, H_0))^{-1}, \\ Q_2(z) &= -H_0 R(z, H_0) Q_1(z) \end{aligned} \tag{2.9}$$

Then if $b<\frac{1}{2}d$ we have

$$\sup_{z\in\Gamma}|\langle f_1, Q_1(z)f_1\rangle|\leqslant 4d^{-2}(1-2b/d)^{-1}b|\Delta V_{11}|, \tag{2.10}$$

$$\sup_{z\in\Gamma}|\langle f_1, Q_2(z)f_1\rangle|\leqslant 8\sum_{i=1}^{2N}\mu_i(2N)^{-1}d^{-3}(1-2b/d)^{-1}b|\Delta V_{11}|, \tag{2.11}$$

$$\sup_{z\in\Gamma}|\langle f_1, Q_1(z)f_k\rangle|\leqslant 4d^{-2}(1-2b/d)^{-1}b|\Delta V_{ii}|^{1/2}|\Delta V_{11}|^{1/2}, \tag{2.12}$$

$$\sup_{z\in\Gamma}|\langle f_i, Q_2(z)f_k\rangle\leqslant 8d^{-2}(2N)^{-1}\sum_{j=1}^{2N}\mu_j(1-2b/d)^{-1}b|\Delta V_{ii}|^{1/2}|\Delta V_{11}|^{1/2} \tag{2.13}$$

whenever $i\neq 1$. (2.12) and (2.13) hold also with i interchanged with k.

Proof. Let us first recall that $\sup_{z\in\Gamma}\|\Delta VR(z, H_0)\|\leqslant b\ \sup_{z\in\Gamma}\|R(z, H_0)\|=2bd^{-1}$. Hence the geometric series $\Sigma_{n=0}^{\infty}\|\Delta VR(z, H_0)\|^n$ is norm convergent to $(1+\Delta VR(z, H_0))^{-1}$, which is therefore bounded by $(1-2bd^{-1})^{-1}$. Hence

$$\begin{aligned}
&\sup_{z\in\Gamma}|\langle f_1, Q_1(z)f_1\rangle|\\
&\qquad=\sup_{z\in\Gamma}\left|\left\langle R(\bar z, H_0)\Delta Vf_1, \sum_{n=0}^{\infty}(\Delta VR(z, H_0))^n\Delta VR(z, H_0)f_1\right\rangle\right|\\
&\qquad<2d^{-1}\|\Delta Vf_1\|(1-2bd^{-1})^{-1}\sup_{z\in\Gamma}\|\Delta VR(z, H_0)f_1\|\\
&\qquad\leqslant 2d^{-1}(1-2bd^{-1})^{-1}\|\Delta Vf_1\|^2\sup_{z\in\Gamma}\left\|\Delta V\sum_{k,j}c_{ik}e_{kj}(\mu_k-z)^{-1}f_j\right\|\\
&\qquad\leqslant 4(1-2bd^{-1})^{-1}\|\Delta Vf_1\|^2
\end{aligned}$$

because $\|\Delta Vf_k\|\leqslant\|\Delta Vf_1\|$ for $\hbar$ small. Here of course $(e_{jk})_{j,k=1}^{2N}=U^{-1}$, $e_{j,k}=\pm(2N)^{-1/2}$. Now $\|\Delta Vf_1\|^2=\int_{a_1^2}^{a_2}|\Delta V|^2|f_1|^2\,dx\leqslant b|\Delta V_{11}|$, whence (2.10). (2.11) is proved in the same way, and so are (2.12), (2.13), with the obvious modification $\|\Delta Vf_i\|\ \|\Delta Vf_1\|\leqslant b^{1/2}|\Delta V_{ii}|^{1/2}b^{1/2}|\Delta V_{11}|^{1/2}$.

Proof of proposition 2.3. Statement (1), i.e. the stability of the band eigenvalues, is a well known consequence of regular perturbation theory (see e.g. Kato (1966, ch II, VII) or Reed and Simon, (1975–8, XII. 1, 2). To see (2), first recall that the strong Riemann integral (Kato 1966, p 67)

$$P_0=(2\pi\mathrm{i})^{-1}\int_\Gamma R(z, H_0)\,\mathrm{d}z,$$

Γ as in 2.4, defines the orthogonal projection on $\mathcal{H}_{2N}$, the $2N$-dimensional subspace spanned by the band eigenvectors $\psi_1,\dots,\psi_{2N}$. A basis in $\mathcal{H}_{2N}$ is equivalently given by $\{f_i\}_{i=1}^{2N}$. As proved in lemma 2.4, the resolvent $R(z, H)$ is bounded uniformly in $z\in\Gamma$, and hence the strong Riemann integral

$$P=(2\pi\mathrm{i})^{-1}\int_\Gamma R(z, H)\,\mathrm{d}z$$

exists and defines the orthogonal projection on the $2N$-dimensional subspace spanned by the eigenvectors $\{\phi_i\}_{i=1}^{2N}$ corresponding to the eigenvalues $\{E_i\}_{i=1}^{2N}$ of H. These eigenvalues of course coincide with the non-zero eigenvalues of the $2N$-rank operator $PHP = HP = PH$. Expand now HP in powers of ΔV up to first order and keep the remainder:

$$\begin{aligned} HP = (H_0+\Delta V)P &= (H_0+\Delta V)(2\pi \mathrm{i})^{-1}\int_\Gamma R(z,H)\,\mathrm{d}z \\ &= H_0(2\pi\mathrm{i})^{-1}\int_\Gamma R(z,H_0)\,\mathrm{d}z - H_0(2\pi\mathrm{i})^{-1}\int_\Gamma R(z,H_0)\Delta V R(z,H_0)\,\mathrm{d}z \\ &\quad +\Delta V(2\pi\mathrm{i})^{-1}\int_\Gamma R(z,H_0)\,\mathrm{d}z + (2\pi\mathrm{i})^{-1}\int_\Gamma Q_1(z)\,\mathrm{d}z \\ &\quad +(2\pi\mathrm{i})^{-1}\int_\Gamma Q_2(z)\,\mathrm{d}z. \end{aligned}$$

The $2N$-rank operator HP can be represented by the matrix $T = (\langle f_i, HPf_k\rangle)_{i,k=1,\dots 2N}$ on the unperturbed basis $\{f_i\}_{i=1}^{2N}$ ($\{f_i\}$ is obtained from $\{\psi_i\}$ through a unitary transformation). We then have, integrating by the residue method the terms up to first order and taking the scalar products,

$$T = T_0 + T_1 + R_1 + R_2$$

where

$$\begin{gathered} T_0 = (\langle f_i, H_0 f_k\rangle)_{i,k=1}^{2N}, \qquad T_1 = (\langle f_i, \Delta V f_k\rangle)_{i,k=1}^{2N}, \\ R_1 = \left((2\pi\mathrm{i})^{-1}\int_\Gamma \langle f_i, Q_1(z) f_k\rangle\,\mathrm{d}z\right)_{i,k=1}^{2N}, \qquad R_2 = \left((2\pi\mathrm{i})^{-1}\int_\Gamma \langle f_i, Q_2(z) f_k\rangle\,\mathrm{d}z\right)_{i,k=1}^{2N}. \end{gathered} \tag{2.14}$$

We have of course

$$\begin{aligned} &\langle f_i, H_0 f_i\rangle = \sum_{k=1}^{2N} c_{ik}^2 \mu_k(\hbar) = \frac{1}{2N}\sum_{k=1}^{2N}\mu_k(\hbar) = \frac{1}{2N}\mathrm{Tr}\,T_0, \\ &\langle f_i, H_0 f_k\rangle = \sum_{j=1}^{N} c_{ij}c_{ik}\mu_j(\hbar), \qquad i \neq k, \\ &|\langle f_i, H_0 f_k\rangle| < \exp[-2(A-\varepsilon_1)/\hbar], \end{aligned} \tag{2.15}$$

by (2.2), (2.4). T_0 has of course eigenvalues $\mu_1, \dots, \mu_{2N}$ and the corresponding eigenvectors are $\{e_{1,i}\}_{i=1}^{2N}, \dots, \{e_{2N,i}\}_{i=1}^{2N}$. The first-order eigenvalues are those of $T_0 + T_1$, and the exact ones those of T. We now have

$$T_{11} = (1/2N)\,\mathrm{Tr}\,T_0 + \Delta V_{11} + (R_1)_{11} + (R_2)_{11}.$$

By lemma 2.4

$$\begin{aligned} |\Delta V_{11}|\{1-4bd^{-2}[1+2\mathrm{Tr}\,T_0(2Nd)^{-1}(1-2bd^{-1})^{-1}]\} &\leqslant |\Delta V_{11} + (R_1)_{11} + (R_1)_{11} + (R_2)_{11}| \\ &\leqslant |\Delta V_{11}|\{1+4bd^{-2}[1+2\mathrm{Tr}\,T_0(2Nd)^{-1}(1-2bd^{-1})^{-1}]\} \end{aligned}$$

whence, by (2.5),

$$\begin{aligned} &\exp[-2(B_1+\eta)/\hbar]\{1-4bd^{-2}[1+2\mathrm{Tr}\,T_0(2Nd)^{-1}](1-2bd^{-1})^{-1}\} \\ &\qquad \leqslant |\Delta V_{11} + (R_1)_{11} + (R_2)_{11}| \\ &\qquad \leqslant \exp[-2(B-\eta)/\hbar]\{1+4bd^{-2}[1-2\mathrm{Tr}\,T_0(2Nd)^{-1}(1-2bd^{-1})^{-1}]\}. \end{aligned}$$

On the other hand, by (2.6) and lemma 2.4 we have, for $i \neq 1$ or $k \neq 1$,

$$|\Delta V_{ik} + (R_1)_{ih} + (R_2)_{ih}| \leqslant \{1 + 4bd^{-2}[1 + \mathrm{Tr}\, T_0(2Nd)^{-1}(1-2bd^{-1})^{-1}]\} \times \exp[-(A+B-2\eta)/\hbar].$$

The matrix elements T_{ik}, $i \neq 1$ or $k \neq 1$, are thus exponentially small with respect to $|\Delta V_{11} + (R_1)_{11} + (R_2)_{11}|$ because $B < B_1 < A$ and we can take $B_1 < (A+B)/2$. It is therefore immediately seen that (2.8) holds.

The exponential localisation of the wavefunction is now expressed as follows.

Corollary 2.5. Let $\phi_1(x, \hbar) = \Sigma_{k=1}^{2N} \beta_{1k} f_k(x)$ be the eigenfunction corresponding to the eigenvalue $E_1(\hbar)$. Then for any given $\delta > 0$, and for $\hbar$ suitably small there is $\varepsilon(\hbar)\downarrow 0$ as $\hbar \downarrow 0$ such that, for all $k \neq 1$,

$$|\beta_{1k}/\beta_{11}| < \exp[-(A - B - \delta - 2\varepsilon)]. \tag{2.16}$$

Proof. The $2N$-vector $\beta = (\beta_{11}, \ldots, \beta_{1,2N})$ is the eigenvector corresponding to $E_1(\hbar)$, i.e. the solution of the homogeneous system

$$(T - E_1(\hbar)I)\beta = 0$$

where I is the identity $2N \times 2N$ matrix, and we can take $\beta_{11} = 1$. Now, as above, we see that $\|R_1\| = \mathrm{O}((b/d^2)|\Delta V_{11}|)$, $\|R_2\| = \mathrm{O}((b/d^2)|\Delta V_{11}|)$ and, consequently,

$$E_1(\hbar) = E_1^{(1)}(\hbar) + \mathrm{O}((b/d^2)|\Delta V_{11}|), \tag{2.17}$$

$E_1^{(1)}(\hbar)$ being the first-order eigenvalue, i.e. the eigenvalue of $T_0 + T_1$ nearest to $E_1(\hbar)$. By lemma 2.2,

$$E_1^{(1)}(\hbar) = (2N)^{-1}\mathrm{Tr}\, T_0 + \Delta V_{11} + \mathrm{O}(\exp[-(A+B-2\varepsilon)/\hbar]). \tag{2.18}$$

On the other hand

$$\beta_{1,k} = M_k \Delta^{-1}, \qquad \Delta = \det(T_{ik} - E_1(\hbar)\delta_{ik}), \qquad i, k = 2, \ldots, 2N,$$

$M_k = \det T'_k$, T'_k being the matrix obtained by $(T_{ik} - E_1(\hbar)\delta_{ik})$, $i, k = 2, \ldots, 2N$, replacing the kth column by $-T_{il}, i = 2, \ldots, 2N$. Now, as above, we have $|T_{ik}| < \exp[-(A+B-2\varepsilon)/\hbar]$ if $i \neq k$, and $\exp[-2(B_1 - \varepsilon)/\hbar] \leqslant |T_{kk} - E_1(\hbar)| \leqslant \exp[-2(B-\varepsilon)/\hbar]$ for $k = 2, \ldots, N$. Hence by (2.5), (2.6), (2.10), (2.11), (2.13) we easily compute

$$\Delta^{-1} \leqslant \exp[(2N-1)(2B_1 - 2\varepsilon)/\hbar],$$

$$M_k \leqslant \exp[-(2N-2)2(B-\varepsilon)/\hbar - (A+B-2\varepsilon)/\hbar]$$

whence (2.16) with $\delta = (4N-2)(B_1 - B)$.

Remarks

(1) The above argument can be easily repeated to show that the eigenfunctions $\phi_2, \ldots, \phi_{2N}$ corresponding to the eigenvalues $E_2(\hbar), \ldots, E_{2N}(h)$ are concentrated outside the first well.

(2) The eigenvalue $E_1(\hbar)$ is the ground state only if $\Delta V < 0$. Therefore we see that the ground state is concentrated in the first well only in this case.

(3) Proposition 2.3 and corollary 2.5 hold true without change for $H_0(\hbar) = \hbar^2 p^2 + V(x)$ acting in $L^2(\mathbb{R})$, $V(x)$ being any symmetric double well potential; i.e. $V(x) \in C^\infty(\mathbb{R})$ fulfils conditions (1)–(2) above and $V(x)\uparrow\infty$ monotonically as $x > 2\pi$.

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Appendix

Let us briefly review for the convenience of the reader the relevant literature in which the proof of proposition 2.1 can be found. Assertion (1) is well known; for a proof see e.g. Reed and Simon (1975–8, theorem X.12). Assertion (2): for the discreteness of the spectrum, see e.g. Reed and Simon (1975–8, theorem XIII. 67): the bound $C_i'\hbar \leq C_i''\hbar$ is an easy consequence of the min–max principle (see e.g. Reed and Simon (1975–8, theorem XIII. 1)) and Temple's inequality (Reed and Simon 1975–8, theorem XIII.5) because the potential is non-negative with a finite number of quadratic zeros. A convenient choice of trial functions is provided by smooth matchings of harmonic oscillator eigenfunctions in each single well. To see (3), (4), (5), consider first remark (3), i.e. the double well. In this case (2.1) and (2.2), i.e. assertion (3), follow from results of Harrell (1980, § III) through the rescaling $x \to \hbar^{1/2}x$, $E \to \mu\hbar^{-1/2}$, for $\beta = \hbar^2$, and through the asymptotic approximation

$$|V(x)-\mu_i|^{1/2} \sim V(x)^{1/2} + \mathrm{O}(\hbar^{1/2}). \tag{A1}$$

Assertion (4) follows by Harrell (1980, theorem 1.12), of course up to the above rescalings. Assertion (5) is once more proved in Harrell (1980, theorem 1.12, § III) up to rescaling and (A1) approximation. We also note that assertions (2) and (3) can be extracted from general results of Simon (1983).

To see (3), (4), (5) in the general case with periodic boundary conditions, remark that the Bloch representation and the $4N\pi$ periodicity immediately yields the following classification (according to non-decreasing energy) for the band eigenfunctions:

$$\begin{aligned}
&\psi_1(x) = u_0(x),\\
&\psi_{2m}(x) = \exp(\mathrm{i}mx/2N)u_{m/2N}(x),\\
&\psi_{2m+1}(x) = \exp(-\mathrm{i}mx/2n)u_{m/2N}(x), \qquad m = 1, \ldots, N-1,\\
&\psi_{2N}(x) = \sin(x/2)u_{1/2}(x),
\end{aligned} \tag{A2}$$

where $u_k(x)$, $0 \leq k \leq \frac{1}{2}$, is a real-valued even function of period 2π which has no zeros. The complex conjugate eigenfunctions $\psi_{2m}(x)$, $\psi_{2m+1}(x)$, $m = 1, \ldots, N-1$, correspond to degenerate eigenvalues (see e.g. Reed and Simon (1975–8), theorem XIII. 91). The real-valued linear combinations ($m = 1, \ldots, N-1$)

$$\left.\begin{aligned}
\phi_{2m}(x) &= \sin(mx/2N)u_{m/2N}(x),\\
\phi_{2m+1}(x) &= \cos(mx/2N)u_{m/2N}(x),
\end{aligned}\right\} \quad m \text{ odd}, \tag{A3}$$

$$\left.\begin{aligned}
\phi_{2m}(x) &= \cos(mx/2N)u_{m/2N}(x),\\
\phi_{2m+1}(x) &= \sin(mx/2N)u_{m/2N}(x),
\end{aligned}\right\} \quad m \text{ even} \tag{A4}$$

fulfil periodic or antiperiodic boundary conditions at $x = 2N\pi$ and can be considered as the top and bottom states of the mth and $(m+1)$th band, respectively, generated by the Schrödinger operator $\hbar^2 p^2 + V(x)$ considered as an operator in $L^2(\mathbb{R})$ with a potential periodic of period $2N\pi$. Recall that in this case (Reed and Simon 1975–8, theorem XIII.91) all gaps between the periodic and antiperiodic states defined by (A3) and (A4) are absent.

Therefore assertions (3), (4), (5) of proposition 2.1 follow directly from the estimates of Harrell (1979) of course up to the above rescaling and to the translation $x \to x - \pi$.

Note added in proof. After submitting this paper for publication we received a preprint by Helffer and Sjöstrand 'Puits Multiples en Limite Semiclassique—II' where applying the techniques of Helffer and Sjöstrand (1983) they reobtain and generalise the results of Jona-Lasinio *et al* (1981). Their paper also covers the situation described in the present article.

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