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Kinetic energy as a perturbation: a convergent algorithm

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Abstract. The potential energy V is placed into the unperturbed Hamiltonian H_0 and the kinetic energy K remains in the perturbation H_1. It is shown that a convergent N/D method, through standard Fredholm determinants, provides suitable matrix elements of an operator such as $H_1+H_1(E-H)^{-1}H_1$. This confirms that the kinetic energy can be used as a perturbation in the Brillouin–Wigner theory.

1. Introduction

As discussed earlier (Giraud 1978, 1982), there is some interest in the situation where an N-particle Hamiltonian $H=K+V$ can be split as a sum $H=H_0+\lambda H_1$ (with $\lambda=1$ physically) of an easily diagonalisable operator H_0 and a semi-positive definite operator H_1. This interest lies in convergence properties of the Brillouin–Wigner perturbation theory, where the perturbed eigenvalues are solutions of the implicit equation

$$E=\varepsilon_0+F(E). \tag{1.1}$$

In (1.1), ε_0 is the ground state energy of H_0, and one selects H_0 so that ε_0 is non-degenerate and the corresponding unperturbed eigenfunction Φ_0 is square integrable and 'very smooth' (i.e. Φ_0 has everywhere derivatives of all orders and is exponentially decreasing at infinity both in coordinate and momentum representation). The function $F(E)$ is a matrix element of the $\mathscr{B}$ operator defined by

$$\mathscr{B}\equiv\lambda H_1+\lambda H_1Q(E-QHQ)^{-1}\lambda H_1, \qquad Q\equiv 1-|\Phi_0\rangle\langle\Phi_0|, \tag{1.2}$$

namely

$$F(E)\equiv F(E,\lambda=1)\equiv\langle\Phi_0|\mathscr{B}|\Phi_0\rangle. \tag{1.3}$$

The positivity of H_1 induces the identity

$$\mathscr{B}=\lambda H_1^{1/2}\{1-\lambda H_1^{1/2}[Q/(E-H_0)]H_1^{1/2}\}^{-1}H_1^{1/2}, \tag{1.4}$$

which relates $\mathscr{B}$ to the resolvent of an auxiliary operator

$$\mathscr{H}\equiv H_1^{1/2}[Q/(E-H_0)]H_1^{1/2}. \tag{1.5}$$

This is known (Baker 1975a, b) to provide a favourable case for the convergence of diagonal Padé approximants. Hence, for a practical calculation of eigenvalues of H, one calculates an even number $2M$ of terms in the perturbation expansion of F

$$F(E)=\sum_{n=0}^{\infty}\left\langle\Phi_0\left|H_1\left(\frac{Q}{E-H_0}H_1\right)^n\right|\Phi_0\right\rangle, \tag{1.6}$$

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and one deduces from these first $2M$ terms the $[M/M]$ Padé approximant $F_M(E)$. This replaces (1.1) by the M-dependent approximation

$$E = \varepsilon_0 + F_M(E). \tag{1.7}$$

The point is, when H_1 is regular or can be regularised in a uniform way, this scheme has been proved (Giraud 1978) to provide, as $M \to +\infty$, a convergent set of increasing lower bounds to the bound state eigenvalues of H. The proof covers the case of the interelectronic repulsion in atomic and molecular physics, and also the case of the hard core internucleonic repulsion in nuclear physics. The scheme summarised by (1.7) thus appears to have a broad range of applications. *But it would be even more useful if kinetic energy, a positive operator K indeed, could be used for* H_1. For that purpose, however, one has to face the fact that K is not a bounded operator.

As shown recently (Giraud 1982), the singularity of K does not prevent the 'Brillouin–Wigner scheme' remaining valid. Two precautions must be taken however. The first consists in defining

$$H_0 \equiv V - \mu|\chi\rangle\langle\chi|, \qquad \mu > 0, \tag{1.8}$$

$$H_1 \equiv K + \mu|\chi\rangle\langle\chi|, \tag{1.9}$$

where the projector $|\chi\rangle\langle\chi|$ and its strength constant μ can be easily adjusted to an arbitrary choice of the unperturbed ground state $|\Phi_0\rangle$ and corresponding eigenvalue ε_0. It is convenient at this stage to assume that V is a 'smooth' local operator $V(r)$ (with derivatives at all order and at most a polynomial increase at infinity). The relation between Φ_0 and χ, namely

$$(H_0 - \varepsilon_0)|\Phi_0\rangle = 0, \tag{1.10a}$$

hence

$$(V - \varepsilon_0)|\Phi_0\rangle = \mu|\chi\rangle\langle\chi|\Phi_0\rangle, \tag{1.10b}$$

then specifies that χ and Φ_0 have the same exponential decrease at infinity and smoothness properties.

The second precaution is needed because the eigenvalues E under study lie in the continuum part of the spectrum of H_0, which has the same continuum as V. Cuts thus occur in the perturbation terms of F, equation (1.6), because of the propagator $(E - H_0)^{-1}$. To bypass these spurious cuts, which are not present in the *sum* $F(E)$ of the full series, one must calculate $F(E)$ with $\operatorname{Re} E < 0$ *and* $\operatorname{Im} E \neq 0$ and one must minimise the modulus of $[E - \varepsilon_0 - F(E)]$. It has indeed been proved that this modulus vanishes when E converges from the upper or lower complex plane towards the discrete, real eigenvalues of H. The square integrable state defined, for E complex, by the equation

$$|\Psi\rangle = |\Phi_0\rangle + [Q/(E - H_0)]H_1|\Psi\rangle = |\Phi_0\rangle + [Q/(E - QHQ)]H_1|\Phi_0\rangle, \tag{1.11}$$

then converges towards the desired eigenstate of H.

The purpose of the present paper is to calculate $F(E)$ when H_1 contains K, equation (1.9). Because E is complex and K singular, it was not proved for K what was obtained for a regular perturbation, namely that $F_M(E)$ converges towards $F(E)$ when $M \to +\infty$. *A fortiori* it was not shown for K that (1.7) generates convergent lower bounds to the discrete eigenvalues of H. The present work, however, will show how $F(E)$ can be reconstructed by a perturbation algorithm, quite analogous to a Padé approximant, namely an N/D method.

The argument goes by two steps. Section 2 introduces a regularisation of K into a bounded operator K_η. This defines an operator $\mathscr{B}_\eta$, and the corresponding function $F_\eta(E)$ can then be calculated by a convergent algorithm. Then § 3 shows that $F(E)$ is the limit of $F_\eta(E)$ when $\eta \to 0$ as long as $\operatorname{Im} E \neq 0$. The numerical example investigated in Giraud (1982) is then revisited and the demanded convergence when $\eta \to 0$ is indeed observed in § 4.

2. Regularisation

In the $3N$-dimensional space, all inessential spin and isospin complications being omitted, let $\boldsymbol{r} \equiv (\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)$ and $\boldsymbol{p} \equiv (p_1, \ldots, p_N)$ denote the N-particle positions and momenta, respectively. The Hamiltonian under consideration is of the form

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{i>j=1}^{N} v_{ij}(\boldsymbol{r}_i - \boldsymbol{r}_j) + \tfrac{1}{2}\omega^2 R_{\mathrm{cm}}^2 m_{\mathrm{cm}}. \tag{2.1}$$

Here the total centre of mass has been constrained in order to remove Galilean degeneracy of the eigenstates, different masses have been allowed for the particles and the local potentials for each pair can differ from one another, but these subtleties can be omitted in the following. More important are the conditions requested for the local and real potentials, namely smoothness (derivability at all orders) and at most a polynomial increase at infinity in coordinate space.

With a suitable mass scaling if necessary, the matrix element of the kinetic energy operator in momentum representation trivially reads

$$\langle \boldsymbol{p}|K|\boldsymbol{p}'\rangle = p^2\, \delta(\boldsymbol{p} - \boldsymbol{p}'). \tag{2.2}$$

The regularisation high-frequency cut-off now considered in this work is taken as

$$\langle \boldsymbol{p}|K_\eta|\boldsymbol{p}'\rangle \equiv p^2 \exp(-\tfrac{1}{4}\eta^2 p^2)\, \delta(\boldsymbol{p} - \boldsymbol{p}'), \qquad \eta > 0. \tag{2.3}$$

This defines an operator K_η whose coordinate representation is now a *bona fide* convolution kernel, uniformly bounded and with derivatives of all orders

$$\langle \boldsymbol{r}|K_\eta|\boldsymbol{r}'\rangle = [\alpha + \beta(\boldsymbol{r} - \boldsymbol{r}')^2] \exp[-(\boldsymbol{r} - \boldsymbol{r}')^2/\eta^2]. \tag{2.4}$$

Here α and β are just trivial N-dependent constants.

The substitution of K_η for K into the definitions of H, H_1, $\mathscr{B}$ and F, respectively, changes nothing to V, H_0, χ, Φ_0, ε_0 but generates new operators and related functions H_η, $H_{1\eta}$, $\mathscr{B}_\eta$ and F_η. The present section deals with the calculation of F_η.

In the same way as

$$F(E) = \langle \Phi_0|H_1|\Psi\rangle \tag{2.5}$$

(see (1.3), (1.2) and (1.11)) one finds

$$F_\eta(E) = \langle \Phi_0|H_{1\eta}|\Psi_\eta\rangle, \tag{2.6}$$

where Ψ_η is the solution of the analogue of (1.11),

$$|\Psi_\eta\rangle = |\Phi_0\rangle + [Q/(E - H_0)]H_{1\eta}|\Psi_\eta\rangle. \tag{2.7}$$

It will now be proved that (2.7) reduces to a Fredholm equation with a bounded, smooth and fast decreasing kernel.

Lemma 1. The square-integrable wavefunction $\chi(\boldsymbol{r})$ is bounded, smooth and exponentially decreasing.

This is a trivial consequence of (1.10*b*) since the local operator $V(\boldsymbol{r})$ has been chosen as smooth without fast increase and $\Phi_0(\boldsymbol{r})$ can be freely chosen in this theory as smooth and fast decreasing.

Lemma 2. For $\operatorname{Im} E \neq 0$, the coordinate representation of $(E-H_0)^{-1}$ is the sum of a multiplicative term and a rank-1 kernel, both term and kernel being bounded and smooth.

This is a consequence of the identity

$$(E-V+\mu|\chi\rangle\langle\chi|)^{-1}=(E-V)^{-1}(1-\gamma^{-1}|\chi\rangle\langle\chi|(E-V)^{-1}), \tag{2.8}$$

where γ is the number

$$\gamma \equiv \mu^{-1}+\langle\chi|(E-V)^{-1}|\chi\rangle. \tag{2.9}$$

Hence

$$\langle\boldsymbol{r}|(E-H_0)^{-1}|\boldsymbol{r}'\rangle=(E-V(\boldsymbol{r}))^{-1}\,\delta(\boldsymbol{r}-\boldsymbol{r}')-\gamma^{-1}\rho(\boldsymbol{r})\rho^*(\boldsymbol{r}'), \tag{2.10}$$

with

$$\rho(\boldsymbol{r})\equiv\chi(\boldsymbol{r})/(E-V(\boldsymbol{r})). \tag{2.11}$$

The denominator $E-V(\boldsymbol{r})$ has a modulus larger than or at most equal to $\operatorname{Im} E$ and, since $\operatorname{Im} E \neq 0$, can generate no singularity. The matrix element $\langle\chi|(E-V)^{-1}|\chi\rangle$ is finite and so is γ^{-1} since $(E-H_0)^{-1}$ exists as E is not in the spectrum of H_0. Smoothness of χ and V and boundedness of χ induce the same properties for ρ.

Lemma 3. The coordinate representation of Q is the sum of the identity and a smooth, bounded, fast decreasing, rank-1 kernel

$$\langle\boldsymbol{r}|Q|\boldsymbol{r}'\rangle=\delta(\boldsymbol{r}-\boldsymbol{r}')-\Phi_0(\boldsymbol{r})\Phi_0^*(\boldsymbol{r}). \tag{2.12}$$

This is again trivial from the very choice of Φ_0.

Lemma 4. For $\operatorname{Im} E \neq 0$ the coordinate representation of $Q(E-H_0)^{-1}$ is the sum of a multiplicative term and a rank-2 kernel, both term and kernel being bounded and smooth.

This is obvious because, as a consequence of (2.12), one finds

$$Q(E-H_0)^{-1}=(E-H_0)^{-1}-|\Phi_0\rangle(E-\varepsilon_0)^{-1}\langle\Phi_0|, \tag{2.13}$$

and one just needs to read again (2.10).

The needed theorem can now be stated.

Theorem 1. For $\operatorname{Im} E \neq 0$ the coordinate representation of $Q(E-H_0)^{-1}H_{1\eta}$ is the sum $A(\boldsymbol{r},\boldsymbol{r}')$ of two bounded and smooth kernels $B(\boldsymbol{r},\boldsymbol{r}')$ and $C(\boldsymbol{r},\boldsymbol{r}')$, the second of them being of finite rank.

Indeed from (2.10) and (2.13) one finds

$$[Q/(E-H_0)]H_{1\eta}=(E-V)^{-1}H_{1\eta}-\gamma^{-1}|\rho\rangle\langle\rho|H_{1\eta}-(E-\varepsilon_0)^{-1}|\Phi_0\rangle\langle\Phi_0|H_{1\eta}. \tag{2.14}$$

then from (1.9) modified by the substitution of K_η for K, this result, (2.14), becomes

$$\begin{aligned}[Q/(E-H_0)]H_{1\eta}=(E-V)^{-1}K_\eta-\gamma^{-1}|\rho\rangle\langle\rho|K_\eta+\gamma^{-1}|\rho\rangle\langle\chi||\rho\rangle\langle\chi|\\ -(E-\varepsilon_0)^{-1}|\Phi_0\rangle\langle\Phi_0|K_\eta-(E-\varepsilon_0)^{-1}\mu\langle\Phi_0|\chi\rangle|\Phi_0\rangle\langle\chi|.\end{aligned} \tag{2.15}$$

The first term on the right-hand side of (2.15) provides the first kernel stated by the theorem,

$$B(\boldsymbol{r},\boldsymbol{r}')\equiv\langle\boldsymbol{r}|(E-V)^{-1}K_\eta|\boldsymbol{r}'\rangle=(E-V(\boldsymbol{r}))^{-1}[\alpha+\beta(\boldsymbol{r}-\boldsymbol{r}')^2]\exp[-(\boldsymbol{r}-\boldsymbol{r}')^2/\eta^2], \tag{2.16}$$

when one has taken advantage of the locality of V and of the kernel definition of K_η, (2.4). Smoothness (and finiteness) properties of this term are just read off (2.16). The last four terms in the RHS of (2.15) make the second kernel C, listed by the theorem, since they are dyadic. Smoothness and finiteness of $\Phi_0(\boldsymbol{r})$, $\chi(\boldsymbol{r})$ and $\rho(\boldsymbol{r})$ have already been stated. The same properties hold for $\langle\Phi_0|K_\eta|\boldsymbol{r}\rangle$ and $\langle\rho_0|K_\eta|\boldsymbol{r}\rangle$, because for instance

$$\langle\rho|K_\eta|\boldsymbol{r}\rangle=\int \mathrm{d}\boldsymbol{r}'\,\rho^*(\boldsymbol{r})\langle\boldsymbol{r}'|K_\eta|\boldsymbol{r}\rangle \tag{2.17}$$

is a trivial convergent convolution by a smooth and exponentially decreasing kernel, see (2.4).

This result, theorem 1, would be sufficient to solve (2.7) by an N/D method (Riesz and Nagy 1955) if the integration domain were finite. With the usual notations for the theory of Fredholm determinants, the solution in coordinate space reads (with $\lambda=1$ for the physical case)

$$\begin{aligned}\Psi_\eta(\boldsymbol{r})=\Phi_0(\boldsymbol{r})+D^{-1}\int \mathrm{d}\boldsymbol{r}'\,\Phi_0(\boldsymbol{r}')\\ \times\left[A(\boldsymbol{r},\boldsymbol{r}')-\lambda\int A\begin{pmatrix}\boldsymbol{r} & \boldsymbol{r}''\\ \boldsymbol{r}' & \boldsymbol{r}''\end{pmatrix}\mathrm{d}\boldsymbol{r}''+\frac{\lambda^2}{2!}\int \mathrm{d}\boldsymbol{r}''\,\mathrm{d}\boldsymbol{r}'''\,A\begin{pmatrix}\boldsymbol{r} & \boldsymbol{r}'' & \boldsymbol{r}'''\\ \boldsymbol{r}' & \boldsymbol{r}'' & \boldsymbol{r}'''\end{pmatrix}-\dots\right],\end{aligned} \tag{2.18}$$

where $A(\boldsymbol{r},\boldsymbol{r}')$ is the coordinate representation of $Q(E-H_0)^{-1}H_{1\eta}$; then

$$A\begin{pmatrix}\boldsymbol{r} & \boldsymbol{r}''\\ \boldsymbol{r}' & \boldsymbol{r}''\end{pmatrix}\equiv\begin{bmatrix}A(\boldsymbol{r},\boldsymbol{r}') & A(\boldsymbol{r},\boldsymbol{r}'')\\ A(\boldsymbol{r}'',\boldsymbol{r}') & A(\boldsymbol{r}'',\boldsymbol{r}'')\end{bmatrix}, \tag{2.19}$$

and so on for the traditional determinants of the method, and finally the Fredholm determinant is

$$D=1-\lambda\int \mathrm{d}\boldsymbol{r}\,A(\boldsymbol{r},\boldsymbol{r})+\frac{\lambda^2}{2!}\int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}'\,A\begin{pmatrix}\boldsymbol{r} & \boldsymbol{r}'\\ \boldsymbol{r} & \boldsymbol{r}'\end{pmatrix}-\dots. \tag{2.20}$$

As the integration domain is infinite, however, additional precautions are in order.

For that purpose, it will first be assumed that $|V(\boldsymbol{r})|$ is short ranged (i.e. it decreases faster than any power of r when $r\to\infty$). This special case excludes harmonic oscillators and Coulomb potentials for instance, but has nonetheless a broad range of interest. Then one finds the following result.

Lemma 5. For $\operatorname{Im} E \neq 0$ and a short-ranged V, the coordinate representation of the subtracted kernel $A_S \equiv Q(E-H_0)^{-1}H_{1\eta} - E^{-1}K_\eta$ is bounded, smooth and short ranged in both variables $\boldsymbol{r}$ and $\boldsymbol{r}'$.

The four dyadics which make the kernel $C(\boldsymbol{r}, \boldsymbol{r}')$ taken from the RHS of (2.15) have already the desired properties. One is only concerned with the subtracted kernel $B_S \equiv B - E^{-1}K_\eta$. From (2.16) one finds

$$EB_S(\boldsymbol{r}, \boldsymbol{r}') = \langle \boldsymbol{r}|[V/(E-V)]K_\eta|\boldsymbol{r}'\rangle = [V(\boldsymbol{r})/(E-V(\boldsymbol{r}))]\langle \boldsymbol{r}|K_\eta|\boldsymbol{r}'\rangle. \tag{2.21}$$

Short range with respect to $\boldsymbol{r}$ is ensured by $V(\boldsymbol{r})$ which appears in the numerator of B_S. Short range with respect to $(\boldsymbol{r}-\boldsymbol{r}')$ is provided by K_η; see again (2.4). The combination of the short ranges with respect to $\boldsymbol{r}$ on one hand, and $(\boldsymbol{r}-\boldsymbol{r}')$ on the other, provides the short range with respect to $\boldsymbol{r}'$.

Corollary to lemma 5. The kernel $B_S(\boldsymbol{r}, \boldsymbol{r}')$ is integrable and square integrable (and actually integrable at all powers larger than 1).

It is now convenient to write (2.7) as

$$(1-E^{-1}K_\eta)|\Psi_\eta\rangle = |\Phi_0\rangle + A_S|\Psi_\eta\rangle, \tag{2.22}$$

where one recognises $A_S \equiv Q(E-H_0)^{-1}H_{1\eta} - E^{-1}K_\eta$, and of course $A_S = B_S + C$ is smooth and short ranged (and thus integrable and square integrable). Equation (2.22) is equivalent to

$$|\Psi_\eta\rangle = (1-E^{-1}K_\eta)^{-1}|\Phi_0\rangle + \mathscr{A}|\Psi_\eta\rangle. \tag{2.23}$$

with $\mathscr{A} \equiv (1-E^{-1}K_\eta)^{-1}A_S$. A last intermediate result will be necessary, namely:

Lemma 6. The coordinate representation of $(1-E^{-1}K_\eta)^{-1}$ is the sum of the identity and a fast decreasing, smooth convolution kernel. Indeed

$$\langle \boldsymbol{r}|(1-E^{-1}K_\eta)^{-1}|\boldsymbol{r}'\rangle = \\ = (2\pi)^{-3N}\int \mathrm{d}\boldsymbol{p}\, \exp[\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{r}-\boldsymbol{r}')]\left(1 + E^{-1}\frac{p^2\exp(-\frac{1}{4}\eta^2p^2)}{1-E^{-1}p^2\exp(-\frac{1}{4}\eta^2p^2)}\right), \tag{2.24}$$

where the denominator of the Gaussian-like integral remains smooth, bounded and non-vanishing, hence changes nothing to range and smoothness properties.

Corollary to lemma 6. The wavefunction $\tilde{\Phi}_0(\boldsymbol{r}) \equiv \langle \boldsymbol{r}|(1-E^{-1}K_\eta)^{-1}|\Phi_0\rangle$ is smooth and fast decreasing.

The case of short range potentials V is thus solved by the following.

Theorem 2. For $\operatorname{Im} E \neq 0$ and short-ranged V, equation (2.23) is a Fredholm equation with a smooth and short range kernel.

Indeed, from lemma 6, the smoothness and short range properties of A_S are not modified by the convolution with the identity and the fast decreasing, smooth convolution kernel brought by $(1-E^{-1}K_\eta)^{-1}$. Integrability of $\mathscr{A}$ at all powers larger or equal to 1 is then automatic.

Substitution of $\mathscr{A}$ for A and $\tilde{\Phi}_0$ for Φ_0 into (2.18)–(2.20) thus solves (2.7) by a convergent algorithm, both the numerator and denominator being entire functions of λ.

It is clear that the conditions of the infinite derivability and fast decrease at infinity which have been imposed upon V can be somewhat relaxed in order to generalise the validity of (2.18)–(2.20) when implemented with $\mathscr{A}$. Other subtractions are also possible and one might for instance consider

$$\mathscr{A}' \equiv [1-(Q/E)H_{1\eta}]^{-1}[Q/(E-H_0)-Q/E]H_{1\eta}. \tag{2.25}$$

Rather than search for the largest class of slow (polynomial?) decreasing potentials which make $\mathscr{A}$ (or $\mathscr{A}'$) sufficiently integrable for (2.18)–(2.20), the case of repulsive potentials increasing like polynomials will now be discussed briefly.

For such repulsive 'polynomial' potentials, the kernel C deduced from the dyadics of (2.15) is again smooth and fast decreasing, thus one need only consider the properties of $B \equiv (E-V)^{-1}K_\eta$. It is clear that if V increases 'fast enough', the coordinate representation of B will be accordingly fast decreasing with respect to both $\boldsymbol{r}$ and $\boldsymbol{r}'$. Indeed, a short range with respect to $(\boldsymbol{r}-\boldsymbol{r}')$ is provided by $\langle \boldsymbol{r}|K_\eta|\boldsymbol{r}'\rangle$ and a complementary decrease is provided directly by $[E-V(\boldsymbol{r})]^{-1}$. Then (2.18)–(2.20) can be used directly with kernel A. The subtraction leading to kernel $\mathscr{A}$ is not necessary in that case.

The one-dimensional oscillator studied in § 4 will provide integrability and square integrability of the kernel A. A detailed discussion and generalisation of this result is not attempted in this paper. The centre-of-mass potential included in (2.1) to avoid, e.g., nuclear spurious states deserves a special comment, however. Since centre-of-mass and internal degrees of freedom are separated physically, one may subtract from K the centre-of-mass kinetic energy and include it inside V, thus H_0. One may also choose Φ_0 (and χ) to factorise into a centre-of-mass Gaussian wavepacket, eigenstate of that modified H_0, and an internal wavefunction. This procedure is extremely familiar and just shifts ε_0 and E by the relevant zero-point energy. Only the internal degrees of freedom will be activated by the perturbation expansion but all calculations will be made in the single particle representation. This is a technical advantage of some significance.

3. Limit of the regularised solution

Practical calculations will truncate (2.18) and (2.20) at some order M and thus generate a Fredholm (not Padé) approximant $F_{M\eta}(E)$ to $F(E)$. The Fredholm theory, with the conditions discussed in § 2, provides that $F_{M\eta}(E) \to F_\eta(E)$ when $M \to +\infty$, namely that there exists an upper bound $\varepsilon(M, E, \eta)$ such that

$$|F_{M\eta}(E)-F_\eta(E)| < \varepsilon(M, E, \eta) \tag{3.1}$$

and

$$\lim_{M\to\infty} \varepsilon(M, E, \eta) = 0. \tag{3.2}$$

Since in practical calculations one considers E to be restricted to some domain of the complex plane, which may be chosen compact, an interesting question is that of a uniform majoration† $\bar{\varepsilon}(M, \eta)$ and even of an even stronger majoration† $\bar{\bar{\varepsilon}}(M)$. Such

† Here $\bar{\varepsilon}(M, \eta) = \sup_E \varepsilon(M, E, \eta)$ and $\bar{\bar{\varepsilon}}(M) = \sup_{E,\eta} \varepsilon(M, E, \eta)$ if such upper bounds are finite.

strong results could be useful for the purpose of the present section, which is to prove that the solutions of the approximate equations

$$E = \varepsilon_0 + F_{M\eta}(E), \tag{3.3}$$

$$E = \varepsilon_0 + F_\eta(E), \tag{3.4}$$

provide information on the solutions of (1.1).

It is known in advance that solutions of (1.1) exist. No *a priori* similar statement is available for (3.3) and (3.4), all the more so because the second technical precaution recalled in § 1 restricts $\operatorname{Im} E$ to be non-zero. Hence the argument will proceed by means of successive inclusions. The scheme is provided by the following definitions.

Definitions. Let ω be a positive number. The domains $\mathscr{D}_1(\omega, M, \eta)$, $\mathscr{D}_2(\omega, \eta)$ and $\mathscr{D}_3(\omega)$ are defined as the loci of the values of E for which, respectively

$$|F_{M\eta}(E) + \varepsilon_0 - E| < \omega, \tag{3.5}$$

$$|F_\eta(E) + \varepsilon_0 - E| < \omega, \tag{3.6}$$

$$|F(E) + \varepsilon_0 - E| < \omega. \tag{3.7}$$

Whenever necessary for $F_{M\eta}$ and/or F_η this definition can be restricted to $\operatorname{Im} E \neq 0$. The closure of these domains may however contain points and/or segments on the real axis.

Since only $F_{M\eta}$ is available practically, one will try to generate a domain $\mathscr{D}_2$ as a limit of domains $\mathscr{D}_1$ when $M \to \infty$, then a domain $\mathscr{D}_3$ as a limit of domains $\mathscr{D}_2$ when $\eta \to 0$. Then a solution of (1.1) is found (Giraud 1982) in the intersection of the domains $\mathscr{D}_3$ when $\omega \to 0$.

Lemma 7. If there exists a domain $\mathscr{D}_1^*(\omega, \eta)$ and an integer M_0 such that for all $M > M_0$ the domains $\mathscr{D}_1(\omega, M, \eta)$ remain included in the domain $\mathscr{D}_1^*(\omega, \eta)$, then $\mathscr{D}_2(\omega, \eta)$ is also included in $\mathscr{D}_1^*(\omega, \eta)$.

This is trivial because for any point outside $\mathscr{D}_1^*$ the relation (3.5) is violated for all $M \geqslant M_0$. Hence the limit F_η of $F_{M\eta}$ violates the relation (3.6) outside $\mathscr{D}_1^*$.

A stronger result would be to include $\mathscr{D}_2(\omega, \eta)$ in a domain $\mathscr{D}_1(\omega', M_0, \eta)$, $\omega' > \omega$. This is possible if a uniform convergence bound $\bar{\varepsilon}(M, \eta)$ can be established, and one finds trivially $\omega' = \omega + \bar{\varepsilon}$. This search for uniform convergence cases raises an interesting problem, which is not discussed in the present paper, however.

In order to relate $\mathscr{D}_2$ to $\mathscr{D}_3$ it is now necessary to establish convergence of F_η towards F when $\eta \to 0$.

The difference of these functions is

$$F(E) - F_\eta(E) = \langle \Phi_0 | \Delta K + H_1 G Q H_1 - (H_1 - \Delta K) G_\eta Q (H_1 - \Delta K) | \Phi_0 \rangle, \tag{3.8}$$

with

$$\Delta K \equiv K - K_\eta, \qquad G \equiv (E - QHQ)^{-1}, \qquad G_\eta \equiv (E - QH_\eta Q)^{-1}.$$

The momentum representation of ΔK is

$$\langle \boldsymbol{p} | \Delta K | \boldsymbol{p}' \rangle = p^2\, \delta(\boldsymbol{p} - \boldsymbol{p}')[1 - \exp(-\tfrac{1}{4}\eta^2 p^2)], \tag{3.9}$$

hence, because $\langle \boldsymbol{p} | \Phi_0 \rangle$ has been selected with a fast decrease as $p \to \infty$, the results:

Lemma 8. The vector $\Delta K|\Phi_0\rangle$ converges *strongly* towards zero when $\eta \to 0$. Indeed

$$\langle\Phi_0|(\Delta K)^2|\Phi_0\rangle = \int_{p\leq\eta^{-1/2}} \mathrm{d}\boldsymbol{p}\, |p^2\Phi_0(\boldsymbol{p})|^2[1-\exp(-\tfrac{1}{4}\eta^2p^2)]^2 + \int_{p>\eta^{-1/2}} \mathrm{d}\boldsymbol{p}\, |p^2\Phi_0(\boldsymbol{p})|^2[1-\exp(-\tfrac{1}{4}\eta^2p^2)]^2. \tag{3.10}$$

The first integral on the RHS of (3.10) is bounded by

$$I_S = [1-\exp(-\tfrac{1}{4}\eta)]^2 \int \mathrm{d}\boldsymbol{p}\, |p^2\Phi_0(\boldsymbol{p})|^2, \tag{3.11}$$

where the fast decrease of Φ_0 makes $p^2\Phi_0(\boldsymbol{p})$ a square integrable function. The second integral is bounded by

$$I_L = \int_{p>\eta^{-1/2}} \mathrm{d}\boldsymbol{p}|\, p^2\Phi_0(\boldsymbol{p})|^2 = \|K|\Phi_0\rangle\|^2 - \int_{p\leq\eta^{-1/2}} \mathrm{d}\boldsymbol{p}|\, p^2\Phi_0(\boldsymbol{p})|^2 \tag{3.12}$$

Both I_S and I_L obviously vanish when $\eta^{-1/2} \to \infty$.

Corollary to lemma 8. Since for $\operatorname{Im} E \neq 0$ the resolvents G and G_η are bounded by $(\operatorname{Im} E)^{-1}$, and since Q is also a bounded operator, the limit of $(F-F_\eta)$ reduces to

$$\lim_{\eta\to 0}[F(E)-F_\eta(E)] = \lim_{\eta\to 0}\langle\Phi_0|H_1(G-G_\eta)QH_1|\Phi_0\rangle. \tag{3.13}$$

Lemma 9. The momentum components of the vector $GQH_1|\Phi_0\rangle$ decrease at least as fast as $p^{-(2+3N/2)}$ when $p\to\infty$.

Let $|X\rangle$ and $|Y\rangle$, respectively, denote the vectors $QH_1|\Phi_0\rangle$ and $GQH_1|\Phi_0\rangle$. By definition $|Y\rangle$ is the solution of

$$(E-H)|Y\rangle = |X\rangle - |\Phi_0\rangle\langle\Phi_0|H|Y\rangle - H|\Phi_0\rangle\langle\Phi_0|Y\rangle + |\Phi_0\rangle\langle\Phi_0|H|\Phi_0\rangle\langle\Phi_0|Y\rangle. \tag{3.14}$$

It is known in advance that $|Y\rangle$ exists and is square integrable since E is not in the spectrum of H ($\operatorname{Im} E \neq 0$). Then $\langle\Phi_0|Y\rangle$ is finite. Furthermore the smoothness and fast decrease of $|\Phi_0\rangle$ makes $H|\Phi_0\rangle$ smooth and fast decreasing. Then $\langle\Phi_0|H|Y\rangle$ exists. Finally $|X\rangle$ is smooth since it contains only $K|\Phi_0\rangle$, $|\Phi_0\rangle$ and $|\chi\rangle$. Therefore the RHS of (3.14) is a finite combination $|Z\rangle$ of smooth and fast decreasing vectors.

Then the identity

$$(E-H)^{-1} = (E-K)^{-1}[1+V(E-H)^{-1}] \tag{3.15}$$

provides that

$$\langle\boldsymbol{p}|Y\rangle = (E-p^2)^{-1}(\langle\boldsymbol{p}|Z\rangle + \langle\boldsymbol{p}|V|Y\rangle). \tag{3.16}$$

The existence and square integrability of $|Y\rangle$ mean that $\langle\boldsymbol{r}|Y\rangle$ is square integrable. Then if V is smooth and bounded in coordinate space, $V(\boldsymbol{r})\langle\boldsymbol{r}|Y\rangle$ is also square integrable, hence $\langle\boldsymbol{p}|V|Y\rangle$ is also a square integrable function decreasing at infinity as fast as $p^{-3N/2}$ at least. The lemma is established since $\langle\boldsymbol{p}|Z\rangle$ already decreases fast when $p\to\infty$. If $V(\boldsymbol{r})$ has a polynomial increase when $r\to\infty$, the lemma is again established if $V|Y\rangle$ can be proved to remain in the Hilbert space of square integrable functions. This is trivial from the confinement properties of such potentials and the

very fast exponential decays of the tails of the square integrable solutions $\langle \boldsymbol{r} | Y\rangle$ they induce.

Lemma 10. The vector $\Delta K | Y\rangle$ converges strongly towards zero when $\eta \to 0$.

The proof resembles that of lemma 8, as

$$\langle Y|(\Delta K)^2|Y\rangle = \int_{p \leq \eta^{-1/2}} \mathrm{d}\boldsymbol{p}\, |p^2\langle \boldsymbol{p}|Y\rangle|^2[1-\exp(-\tfrac{1}{4}\eta^2 p^2)]^2$$
$$+ \int_{p > \eta^{-1/2}} \mathrm{d}\boldsymbol{p}\, |p^2\langle \boldsymbol{p}|Y\rangle|^2[1-\exp(-\tfrac{1}{4}\eta^2 p^2)]^2. \tag{3.17}$$

From (3.16) and the choice of Re $E<0$ one finds that

$$|p^2\langle \boldsymbol{p}|Y\rangle| < |W(\boldsymbol{p})|, \tag{3.18}$$

where

$$W(\boldsymbol{p}) \equiv \langle \boldsymbol{p}|Z\rangle + \langle \boldsymbol{p}|V|Y\rangle, \tag{3.19}$$

is a square integrable function. Then the first integral in the RHS of (3.17) can be bounded by

$$I'_{\mathrm{S}} = [1-\exp(-\tfrac{1}{4}\eta)]^2 \int \mathrm{d}\boldsymbol{p}\, |W(\boldsymbol{p})|^2, \tag{3.20}$$

and the second integral by

$$I'_{\mathrm{L}} = \|W\|^2 - \int_{p \leq \eta^{-1/2}} \mathrm{d}\boldsymbol{p}\, |W(\boldsymbol{p})|^2. \tag{3.21}$$

The limit of both I'_{S} and I'_{L} is trivially zero when $\eta \to 0$.

The final result can now be stated.

Theorem 3. When $\eta \to 0$, $F_\eta(E)$ converges towards $F(E)$. Indeed from (3.13) one derives

$$\lim(F-F_\eta) = \lim\langle \Phi_0|H_1 Q G_\eta Q \Delta K Q G Q H_1|\Phi_0\rangle, \tag{3.22}$$

and then, by Schwarz's inequality and the commutation of Q with G and G_η

$$|\langle X|G_\eta \Delta K|Y\rangle| \leq (\mathrm{Im}\, E)^{-1}\|X\|\|\Delta K|Y\rangle\|. \tag{3.23}$$

As shown by lemma 10, this vanishes when $\eta \to 0$.

Corollary to theorem 3. If a domain $\mathscr{D}^{**}(\omega)$ contains all domains $\mathscr{D}_2(\omega, \eta)$ when $\eta < \eta_0$, it contains $\mathscr{D}_3(\omega)$. If $\mathscr{D}^{**}(\omega)$ contains all domains $\mathscr{D}_1(\omega, M, \eta)$ for $M > M_0$ and $\eta < \eta_0$ it also contains $\mathscr{D}_3(\omega)$. This is because any point outside of $\mathscr{D}^{**}$ will violate inequalities (3.5) and (3.6), thus their limits when $M \to \infty$ *then* $\eta \to 0$.

In conclusion of this section, it has been proved that $F(E)$ can be calculated as the limit of $F_\eta(E)$. This completes the result of § 2 where it was proved that $F_\eta(E)$ can be calculated as the limit of $F_{M\eta}(E)$.

4. Numerical application

4.1. Technical details

The one-dimensional oscillator $H = x^2 - \mathrm{d}^2/\mathrm{d}x^2$ is considered again, and regularised as

$$H_\eta = V + \lambda K_\eta + (\lambda - 1)\mu|\chi\rangle\langle\chi|. \tag{4.1}$$

For obvious technical reasons it is here useful to operate in momentum representation, where K_η now appears as a short range potential and V as a pseudo kinetic energy. The ground state Φ_0 of H_0 is again selected as

$$|\Phi_0\rangle = (1/\sqrt{2})(|1\rangle + |0\rangle), \tag{4.2}$$

with a slight change in the definition of the phase of the eigenvectors $|0\rangle$, $|1\rangle$, etc of H, in order to have all their wavefunctions real in momentum space. Hence one selects

$$\langle p|\Phi_0\rangle = (1/\sqrt{2})\pi^{-1/4}(1+\sqrt{2}p)\exp(-p^2/2), \tag{4.3}$$

and $\chi = (V - \varepsilon_0)\Phi_0$ such as

$$\langle p|\chi\rangle = (1/\sqrt{2})\pi^{-1/4}(-\sqrt{2}p^3 - p^2 + 3\sqrt{2}p + 1 - \varepsilon_0\sqrt{2}p - \varepsilon_0)\exp(-p^2/2). \tag{4.4}$$

This phase modification changes nothing to the earlier result (Giraud 1982)

$$F(E) = 2 - \varepsilon_0 + (E-2)^{-1}, \tag{4.5}$$

and the arbitrariness of $\varepsilon_0 < 0$ with $\mu = (1-\varepsilon_0)^{-1}$.

In this one-dimensional model it is trivial to check that the kernel B, equation (2.16), reads

$$B(x, x') = (E - x^2)^{-1}K_\eta[(x-x')/\eta], \tag{4.6}$$

and is thus integrable and square integrable. This makes both $[Q(E-H_0)^{-1}H_{1\eta}]$ and $[H_{1\eta}Q(E-H_0)^{-1}]$ trace operators and Hilbert–Schmidt operators. A solution of (2.7) by Fredholm approximants (N/D method) is then possible. Alternatively, since the regularisation of K into K_η retains the positivity of K, the perturbation $H_{1\eta}$ has the same positivity. Hence an equivalent of (1.5) exists and defines $\mathscr{H}_\eta$, and furthermore, because of cyclic invariance of the trace, the number $\mathrm{Tr}\,\mathscr{H}_\eta = \mathrm{Tr}[Q/(E-H_0)]H_{1\eta}$ is finite and the number

$$\mathrm{Tr}\,\mathscr{H}_\eta^\dagger\mathscr{H}_\eta = \mathrm{Tr}[Q/(E^*-H_0)]H_{1\eta}[Q/(E-H_0)]H_{1\eta} \tag{4.7}$$

is also finite from Schwarz's inequality applied to the scalar product of Hilbert–Schmidt operators.

In this application we do not elaborate longer on the Fredholm manipulation of (2.7), for it is easy in the present case to solve (2.7) directly. For it has been shown to be equivalent to

$$(E - H_\eta)|\Psi_\eta\rangle = D(E)|\Phi_0\rangle, \tag{4.8}$$

where, as a matter of fact,

$$D(E) = E - \varepsilon_0 - F_\eta(E). \tag{4.9}$$

It is therefore sufficient to define $\bar{\Psi}_\eta$ as the solution of

$$(E - H_\eta)|\bar{\Psi}_\eta\rangle = |\Phi_0\rangle, \tag{4.10}$$

the renormalisation coefficient $D(E)$ being adjusted to the condition $\langle\Phi_0|\Psi_\eta\rangle=1$ provided by (2.7), hence

$$D(E)=[\langle\Phi_0|\bar{\Psi}_\eta\rangle]^{-1}. \tag{4.11}$$

There are several ways to solve (4.10). Since it also reads

$$(E-V-\lambda K_\eta)|\bar{\Psi}_\eta\rangle=|\Phi_0\rangle+\Delta(E)|\chi\rangle, \tag{4.12}$$

with

$$\Delta(E)=(\lambda-1)\mu\langle\chi|\bar{\Psi}_\eta\rangle, \tag{4.13}$$

one may solve the two differential equations

$$[E+\mathrm{d}^2/\mathrm{d}p^2-\lambda p^2\exp(-\tfrac{1}{4}\eta^2p^2)]\Psi_i(p)=\begin{Bmatrix}\langle p|\Phi_0\rangle\\ \langle p|\chi\rangle\end{Bmatrix}, \tag{4.14}$$

where the index $i=1, 2$ refers to Φ_0 and χ on the RHS, respectively. The boundary conditions for Ψ_1, Ψ_2 are of course those of square integrability. Then $\Delta(E)$ is found from (4.13) itself by

$$\Delta(E)=(\lambda-1)\mu[\langle\chi|\Psi_1\rangle+\Delta(E)\langle\chi|\Psi_2\rangle]. \tag{4.15}$$

Rather than using (4.14) the present calculation is based on a matrix approximation to (4.10). A set of basis functions $\Gamma_i(p)$ $i=1,\ldots,\mathcal{M}$ is chosen, and $\bar{\Psi}_\eta$ is expanded as

$$|\bar{\Psi}_\eta\rangle=\sum_{i=1}^{\mathcal{M}} c_i|\Gamma_i\rangle, \tag{4.16}$$

the coefficient c_i obeying the conditions

$$\sum_i\langle\Gamma_j|(E-H_\eta)|\Gamma_i\rangle c_i=\langle\Gamma_j|\Phi_0\rangle. \tag{4.17}$$

This method is normally not the best to be used in the present case, because the reconstruction of the unbounded operator H_η by finite matrices may raise convergence problems, all the more so because the 'basis' $\{\Gamma\}$ used in the following is a set of displaced Gaussians (in momentum space, with a width σ)

$$\Gamma_i(p)\equiv\pi^{-1/4}\sigma^{-1/2}\exp[-(p-k_i)^2/2\sigma^2]. \tag{4.18}$$

Indeed this 'basis' is not orthonormal and the Gram–Schmidt overlap matrix

$$N_{ji}\equiv\langle\Gamma_j|\Gamma_i\rangle=\exp[-(k_j-k_i)^2/4\sigma^2] \tag{4.19}$$

is known to be ill conditioned. Nonetheless the experience gained in the generator coordinate theory of nuclear reactions (Wong 1975, Le Tourneux 1978) shows that an accurate numerical solution of this generalised Griffin–Hill–Wheeler equation (Griffin and Wheeler 1957, Hill and Wheeler 1953)

$$\sum_i(EN_{ji}-H_{ji})c_i=d_j \tag{4.20}$$

is possible. Here, with obvious notations

$$H_{ji}=V_{ji}+\lambda K_{ji}+(\lambda-1)\mu\chi_j\chi_i, \tag{4.21}$$

$$V_{ji}\equiv\langle\Gamma_j|V|\Gamma_i\rangle=N_{ji}[1/2\sigma^2-(k_j-k_i)^2/4\sigma^4], \tag{4.22}$$

$$K_{ji}\equiv\langle\Gamma_j|K_\eta|\Gamma_i\rangle=\frac{\bar{\sigma}}{\sigma}N_{ji}\left(\frac{\bar{\sigma}^2}{2}+\frac{(k_j+k_i)^2\bar{\sigma}^4}{\sigma^4}\right)\exp\left[-\frac{(k_j+k_i)^2}{4\sigma^2}\left(1-\frac{\bar{\sigma}^2}{\sigma^2}\right)\right], \tag{4.23}$$

with

$$\bar{\sigma}^{-2} = \sigma^{-2} + \tfrac{1}{4}\eta^2; \tag{4.24}$$

then

$$d_j \equiv \langle \Gamma_j | \Phi_0 \rangle = 2^{-1/2}\sigma_0\sigma^{-1/2}\left(1 + 2^{1/2}\frac{k_j}{1+\sigma^2}\right)\exp\left(-\frac{k_j^2}{2+2\sigma^2}\right), \tag{4.25}$$

with

$$\sigma_0^{-2} = \tfrac{1}{2} + 1/2\sigma^2, \tag{4.26}$$

and finally

$$\chi_j \equiv \langle \Gamma_j | \chi \rangle = 2^{-1/2}\sigma_0\sigma^{-1/2}\exp[-k_j^2/(2+2\sigma^2)]$$
$$\times\left(-\sqrt{2}\frac{k_j^3}{(1+\sigma^2)^3} - 3\sqrt{2}\frac{k_j}{1+\sigma^2}\left(\frac{1}{2} - \frac{1}{1+\sigma^2}\right) - \frac{k_j^2}{(1+\sigma^2)^2} - \frac{1}{2} + \frac{1}{1+\sigma^2}\right.$$
$$\left. + (\tfrac{3}{2} - \varepsilon_0)\sqrt{2}\frac{k_j}{1+\sigma^2} + \tfrac{1}{2} - \varepsilon_0\right). \tag{4.27}$$

4.2. Results

In this numerical application the value $\varepsilon_0 = -0.5$, far enough from the final eigenvalues 1 and 3, has been selected. Various widths σ for the basis, (4.18), have been considered,

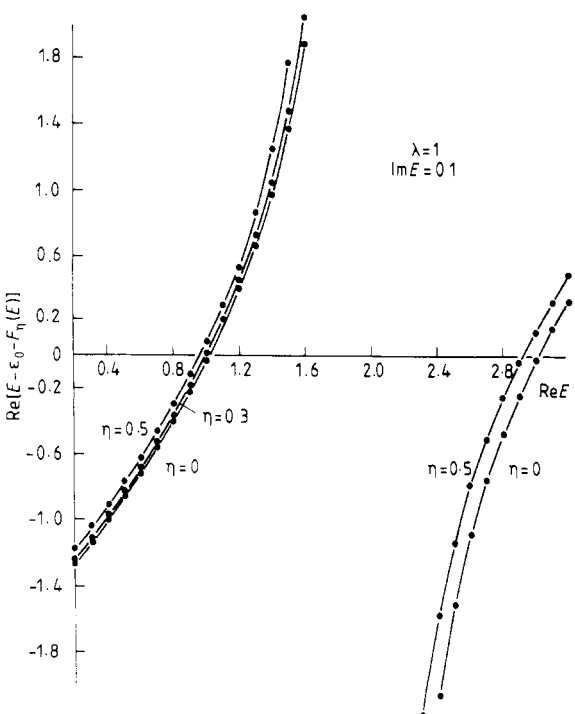

Figure 1. Behaviour of the Brillouin–Wigner equation. The value $\eta = 0$ corresponds to the exact Hamiltonian. The value $\eta = 0.5$ corresponds to a very strong cut-off of the perturbation. Because of the observed strong convergence as $\eta \to 0$, the intermediate value $\eta = 0.3$ is shown only in the left part of the plot. It is remarkable that for a small imaginary part of E, Im $E = 0.1$, the bundle of curves does cross the axis at $E = 1$ and $E = 3$.

with a typical value $\sigma = 1$. Various step sizes in the mesh made by the k_i, equation (4.18), have also been considered, with a typical minimal distance between wavepackets $k_{i+1} - k_i = 1$. Finally various basis dimensions, ranging from 30 to 70, have also been investigated. Numerical stability has been obtained and the values of Re $D(E)$ for $\eta = 0$, $\eta = 0.3$ and $\eta = 0.5$ are displayed as functions of Re E in figure 1 when Im $E = 0.1$.

It is extremely striking that for $\eta = 0.5$, which is a very strong cut-off of K, the values reached for Re $D(E)$ are extremely close to those of the exact case $\eta = 0$. As a check of this strong convergence, the curve for $\eta = 0.3$ perfectly interpolates between $\eta = 0.5$ and $\eta = 0$. It can be stressed, finally, that Re $D(E)$ vanishes for values of Re E which are very close to the expected eigenvalues 1 and 3.

The numerical plot suggests furthermore that the cancellation of Re $D(E)$ for $\eta > 0$ may provide lower bounds to the exact eigenvalues, a likely consequence of the positivity of the perturbation K_η and of the operator inequality $K_\eta < K$, but this has not been established as a theorem (all the more so Im E is small, but not zero). The conjecture defines an interesting line of investigation, however.

5. Discussion and conclusion

Two main results have been obtained, namely: (i) the kinetic energy operator can be used as a perturbation, provided a high frequency cut-off is implemented, and (ii) individual matrix elements of the resolvent of this regularised operator have a smooth limit when the cut-off is removed.

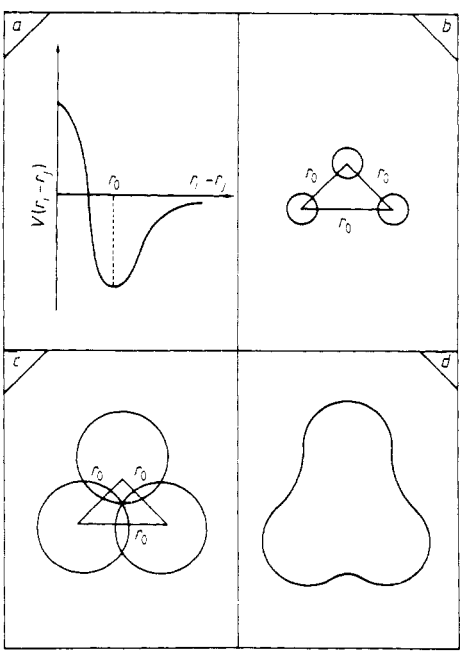

Figure 2. (Schematic). (*a*) shows a two-body potential with an equilibrium distance r_0. (*b*) shows three narrow wavepackets localised at that distance from each other. In (*c*) the kinetic energy increases the width of the wavepackets. In (*d*) the packets have fused but retain part of the classical limit geometry.

An inconvenience of the theory, however, is the use of a Fredholm algorithm because multi-dimensional integrations such as demanded by (2.18) and (2.20) tend to be unwieldy. Fast algorithms for the calculation of $F(E)$ would be of significant use in making the theory more useful. In that sense, Padé approximants might be investigated in order to take advantage of the positivity of K and the integrability of the kernels found in the theory, as recomended by Chisholm (1970).

One of the main applications of the theory which can be advocated is as follows. Assume that the interaction $V(\boldsymbol{r}_i - \boldsymbol{r}_j)$ of the finite system of N particles under study has a minimum at some classical equilibrium distance r_0 (see figure 2(a)). This is a situation more than often met in molecular, atomic or nuclear physics. When Planck's constant is extremely small, the particles tend to localise in narrow wavepackets locating from each other as much as possible at this equilibrium distance, in order to minimise the potential energy. Such a model of a finite crystal can be selected as the unperturbed state Φ_0 (figure 2(b)). Then as $\hbar$, the coupling constant of K, is turned on, kinetic energy increases, the wavepackets must grow and start overlapping (figure 2(c)). Although finite systems do not show sharp phase transitions, a melting of the crystal must be observed about some critical range of $\hbar$. The parameters and geometry of the resulting shape of the system (figure 2(d)) should then give some understanding of the collective degrees of freedom of the system. The present theory thus looks like a constructive derivation of these collective phenomena shown by finite quantum systems when $\hbar$ reaches its physical value.

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