CONVERGENCE OF TIME DEPENDENT PERTURBATION THEORY FOR AUTOIONIZING STATES OF ATOMS‡

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We give a rigorous proof of the convergence of the formulae from time dependent perturbation theory in a variety of cases including Auger states.

The convergence of time independent perturbation theory for isolated levels of quantum mechanical system is an old result [1] *. But convergence (or even the precise rigorous meaning) of time dependent perturbation series has resisted proof for over thirty years **. In this note we wish to sketch a method of proving convergence of the time dependent series in a variety of cases including autoionizing states in atoms. The fuller details will be discussed elsewhere [4]. Our basic technique is due to Balslev and Combes [5] who invented it to solve another problem.

Let us describe the method in a special case. Consider a helium atom Hamiltonian without relativistic corrections, in the limit of infinite nuclear mass and with the Coulomb repulsion between electrons turned off, i.e.

$$H_0 = -\Delta_1 - \Delta_2 - 2/r_1 - 2/r_2$$

as an operator on $L^2(\mathbf{R}^6)$. H_0 has eigenvalues at $\{-1/n^2 - 1/m^2\}_{n,m=1}^{\infty}$ and continuous spectrum beginning at -1. Thus the eigenvalues $E_{n,m} = -(n^{-2} + m^{-2})$ are embedded in the continuum if $n,m \geq 2$. Now let us consider the Hamiltonian $H_0 + \beta V$ with $V = |\boldsymbol{r}_1 - \boldsymbol{r}_2|^{-1}$. The eigenvalues embedded in the continuum turn into resonances whose widths are given by time dependent perturbation series. It is these series for which we will prove convergence. We deal with channels in which $E_{n,m}$ is non-degenerate †.

Let $U(\theta)$ be the scaling operators on $L^2(\mathbf{R}^6)$, i.e. $(U(\theta)\psi)(\boldsymbol{r}) = e^{3\theta}\psi(e^{\theta}\boldsymbol{r})$. Define $H_0(\theta) \equiv U(\theta)\, H_0\, U(\theta)^{-1} = e^{-2\theta}(-\Delta_1 - \Delta_2) - e^{-\theta}(2/r_1 + 2/r_2)$; $V(\theta) \equiv U(\theta)\, V U(\theta)^{-1} = e^{-\theta} V$; $H(\theta;\beta) = H_0(\theta) + \beta V(\theta)$. While $U(\theta)$ is only defined for θ real, $H_0(\theta)$ and $H(\theta;\beta)$ have a natural analytic continuation into the strip $|\mathrm{Im}\theta| < \frac{1}{4}\pi$. By results of Balslev and Combes [5], $H_0(\theta)$ has a very simple spectrum. First, its eigenvalues are those of H_0 ††, but the essential spectrum of $H_0(\theta)$ is $\{-1/n^2 + e^{-2\theta}\lambda \mid \lambda \in [0,\infty];\ n = 1,2 \dots \infty\}$ †††. Moreover, by other results of Balslev and Combes [5], $\langle \psi, (H_0 + \beta V - Z)^{-1}\psi \rangle = f_4(Z)$ has an analytic continuation onto a second sheet on a dense set of $\psi \in L^2(\mathbf{R}^6)$ with singularities only at eigenvalues of $H(\theta;\beta)$ where there are poles, and branch points at certain "complex thresholds".

Now, we first notice $E_{n,m}$ are isolated eigen-

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* For results on the meaning of divergent time independent perturbation series, see ref. [2].

** For some attempts at studying related phenomena in models see ref. [3].

† For example, if $n = m = 2$ and $^{2S+1}L(P)$ indicates L = angular momentum, P = parity, S = total electron spin or equivalently symmetry of the wave function there is one $^1D^{(+)}$, one $^3P^{(+)}$, one $^3P^{(-)}$, one $^1P^{(-)}$ and two $^1S^{(+)}$ states. Both H_0 and V preserve L, P and S and we can restrict ourselves to subspaces of states of good L, m_L, S, m_S and P. The $D^{(+)}$ and $^{1,3}P^{(-)}$ states are non-degenerate and turn into resonances. The $^3P^{(+)}$ state is not embedded in a $P^{(+)}$-continuum, since all continuum states of energy below $-1/4$ have natural parity. It does not turn into a resonance. The two $^1S^{(+)}$ states are degenerate and are not treatable by the method sketched in this paper. If the degeneracy is broken in first or second order though, analyticity can be proven by a modified method [4].

†† The eigenvalues of $H_0(\theta)$ are analytic in θ but constant for θ real since $H_0(\theta) = U(\theta) H_0 U(\theta)^{-1}$ if θ is real.

††† The special role played by n^{-2} is due to the fact that they are the thresholds of H_0, i.e. bound state energies of two body subsystems.

values of $H_0(\theta)$ if Im $\theta > 0$. Thus if we deal with non-degenerate channels †, $H_0(\theta)+\beta V(\theta)$ has a single eigenvalue, $E(\beta)$, (In the channel in question) near $E_{n,m}$ for β small and $E(\beta)$ is analytic at $\beta = 0$. By the usual time independent theory, $E(\beta)$ has a convergent power series expansion near $\beta = 0$ with terms given by the usual Rayleigh-Schrödinger formulae (with modifications due to the non-self adjoint nature of $H_0(\theta)$ and $V(\theta)$ when Im $\theta > 0$). In particular, the "width" of $E(\beta)$:

$$\Gamma(\beta) = i[E(\beta) - \overline{E(\bar{\beta})}]$$

is analytic at $\beta = 0$. Since $\Gamma(\beta) \geq 0$ for β real ‡ $\Gamma(\beta) = a_2\beta^2 + \dots$. Detailed analysis shows [4] that a_2 is given by the Fermi-Goldon rule and the higher orders by formulae of the time dependent formalism. We thus have a convergent power series expansion for the widths of autoionizing levels ‡‡.

These results extend immediately to a larger class of systems. Combes [3] introduced a class of potentials called dilatation analytic potentials. Combes' class includes certain spin orbit and non-local interactions but the local central potentials in Combes' class are precisely [4] the functions $V(r)$ with analytic continuations, $V(Z)$, to the sector $\{z \mid |\arg z| < \alpha\}$ for some $\alpha > 0$ obeying $\lim_{Z\to\infty;\ |\arg Z| < \alpha - t} |V(Z)| = 0$ and a local L^2-condition for $V(re^{i\beta})$ as functions on $\mathbf{R}^3$. In particular, Combes' class includes sums of Yukawa and $r^{-\delta}$ potentials if $0 < \delta < 3/2$. Let $H_0 = -\Delta_1 - \dots -\Delta_{n-1} + \sum_{i=1}^n W_{i0}(r_i) + \sum_{i<j} W_{ij}(r_{ij})$, $V = \sum_{i=1}^n V_{i0}(r_i) + \sum_{i<j} V_{ij}(r_{ij})$. Here all the V's and W's are in Combes' class. If H_0 has a non-degenerate eigenvalue embedded in its continuum at a non-threshold value, the width of the resonance of $H_0+\beta V$ near this eigenvalue is given by a convergent series.

In this way one can prove the convergence of the series of time dependent perturbation series.

† See footnote † on previous page.

‡ One proves [4], if $\Gamma(\beta) < 0$, $H_0+\beta V$ would have a complex eigenvalue.

‡‡ We emphasize that we don't know that the physical value $\beta = 1$ is in the circle of convergence for $\Gamma(\beta)$.

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