

Some remarks on approximation methods for quantum systems in higher space dimensions

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ABSTRACT

We consider the effect of space dimension N , on the results predicted by two approximation techniques applied on physical quantum systems. In the first, we apply degenerate perturbation theory to perturbed N -dimensional infinite cubical well. It is found that the energy difference for splitting decreases as N increases and it vanishes in the infinite dimensional space. In the second, we apply the sudden approximation to the electronic structure change implied by beta-decay of the tritium nucleus. It is found that as N increases the ionization probability increases.

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INTRODUCTION

Approximation methods are of great importance and widely used in quantum mechanics and have been enormously successful in obtaining approximate solutions to quantum systems. These methods, for both stationary problems and time-dependent problems, are usually applied to quantum systems in space dimension $N \leq 3$. Over the past two decades, the generalization of the three-dimensional problems to higher dimensions received a considerable development mathematical and theoretical physics. For example, the N -dimensional analogy of the hydrogen atom has been investigated extensively over the years (Avery and Herschbach, 1992), (Kirchberg et al., 2003), (Saelen et al., 2007). In addition, the generalization to higher dimensions is useful in random walks (Mackay et al., 2002), in Casimir effect (Bender et al., 1992), in harmonic oscillator (Oyewumi et al., 2008), (AL-Jaber, 2008), (Rothos et al., 2009), and in mathematical physics (Bredies, 2009), (Szymtkowski, 2007), (Bouda and Ghabri, 2008), (Golovnev, 2006). It is interesting to expose undergraduate students to simple, but illustrative, quantum systems in higher space dimensions. Therefore, it is tempting to apply specific approximation methods to certain quantum systems in N -dimensional space. It must be emphasized that our intention here is not to find approximate solutions but rather to expose the reader to higher dimensional problems and to examine the effect of the space dimension on the results of two well-known approximation methods in quantum mechanics. We choose two approximation methods, one for stationary quantum system and another for time-dependent one. For the first method, we consider the time-independent degenerate perturbation theory applied to N -dimensional infinite cubical well that is perturbed with some perturbation, H' . The reason behind the selection of degenerate perturbation theory lies on its wide recent applications in various settings: In studying degeneracy breaking due to short-ranged impurities in atomically doped Carbon nanotubes (Bondarev and Lambin, 2005), (McCann and Fal'ko, 2005), in

investigating the effects of magnetic anisotropy in magnetic molecules (Kostantinidis and Coffey, 2002), (Meng and Wessel, 2008), (Bialynicki and Sowinski, 2007), (Bergman et al., 2007), in discussing quantum systems coupled to oscillators (Muthukumar and Mitra, 2002), (Hagelstein et al., 2008), in dealing with many-body interacting systems (Stauber et al., 2000), (Morawetz, 2002), in studying degenerate atomic systems (Vilain et al., 2001), and in calculating relativistic corrections for low-lying excited states when a hydrogen atom is placed in a strong magnetic field (Poszwa and Rutkowski, 2004). For the second method we choose the sudden approximation and apply it to β -decay of Tritium atom. The sudden approximation has been widely used for describing abrupt change in the Hamiltonian of the system. For example, some workers used the sudden approximation in calculating photo-ionization cross section of atoms induced by strong fields (Kazansky and Kabachnik, 2007), (Ydin et al., 2007). Others applied this method in the study of the multiple electron loss of heavy projectiles in fast ion-atom collisions (Matveev et al., 2009), (Voitkiv et al., 1999), (Salop and Eichler, 1979), (Richards, 1981), (Kapusta and Mocsy, 1999). In addition, there has been an investigation, using sudden approximation, on how hydrogen atoms respond to perturbation by intense ultrafast laser pulses of duration shorter than the inverse of the initial-state energy (Lugovskoy and Bray, 2006), (Lugovskoy and Bray, 2005). More interestingly, the sudden approximation has been used in the calculations of transition probabilities of electronic excitations resulting from β -decay in atomic processes (Frolov and Talman, 2005), (Saenz and Froelich, 1997), (Froelich and Saenz, 1996), (Wauters and Vaeck, 1996), (Claxton et al., 1992). The organization of the present paper goes as follows: In section 1, we give an introduction. Section 2 deals with degenerate perturbation theory applied to a perturbed N -dimensional infinite cubical well. In section 3, the sudden approximation method is applied to the process of β -decay of Tritium atom in N dimensions. Section 4 is devoted for results and conclusions.

Perturbed N -dimensional infinite cubical well

We consider an infinite cubical well of side a in N space dimensions whose potential is given by

$$V(x_1, x_2, x_3, \dots, x_N) = \begin{cases} 0 & 0 < x_i < a \quad i = 1, \dots, N \\ \infty & \text{otherwise} \end{cases} \quad (1)$$

The stationary states solutions for Schrödinger equation are

$$\psi_{n_1, n_2, \dots, n_N}(x_1, x_2, \dots, x_N) = \left(\frac{2}{a}\right)^{\frac{N}{2}} \prod_{i=1}^N \text{Sin}\left(\frac{n_i \pi x_i}{a}\right), \quad (2) \quad \text{with } n_i \text{ a}$$

positive integer for all values of i . The corresponding allowed energies are

$$E^0 = \frac{\pi^2 \hbar^2}{2ma^2} \sum_{i=1}^N n_i^2. \quad (3)$$

Notice that the ground state ($\psi_{1,1,1,\dots,1}$) is non-degenerate with energy

$$E_0^0 = \frac{N\pi^2 \hbar^2}{2ma^2}. \quad (4)$$

Since we are interested in the effect of space dimension on splitting degenerate states, we need to consider the first excited state which is N degenerate, namely

$$\psi_{1,1,1,\dots,2}, \psi_{1,1,1,\dots,2,1}, \psi_{1,1,1,\dots,2,1,1}, \psi_{1,1,1,\dots,2,1,1,1}, \dots, \psi_{2,1,1,\dots,1}, \quad (5)$$

all have the same (unperturbed) energy, which is

$$E_1^0 = \frac{\pi^2 \hbar^2}{2ma^2} \left(4 + \sum_{i=1}^{N-1} 1\right) = (N+3) \frac{\pi^2 \hbar^2}{2ma^2}. \quad (6)$$

We introduce the perturbation

$$H' = \begin{cases} V_0 & 0 < x_i < \frac{a}{2} (i = 1, 2, \dots, N-1) \\ 0 & \dots \dots \dots \text{otherwise} \end{cases} \quad (7)$$

We now construct the matrix W , whose elements are the matrix elements W_{ij} of H' with respect to the unperturbed wave functions $\psi_1, \psi_2, \dots, \psi_N$, with

$$\psi_i = \psi_{111\dots(N-i)\text{times}, 2, 11\dots(i-1)\text{times}} \quad (8)$$

$$W_{ij} = \langle \psi_i | H' | \psi_j \rangle \quad (9)$$

The diagonal elements are

$$W_{ii} = \left(\frac{2}{a}\right)^N V_0 \int_0^a \text{Sin}^2\left(\frac{\pi x_N}{a}\right) dx_N \int_0^{a/2} \text{Sin}^2\left(\frac{2\pi x_i}{a}\right) dx_i \prod_{\substack{j=1 \\ j \neq i}}^{N-2} \int_0^{a/2} \text{Sin}^2\left(\frac{\pi x_j}{a}\right) dx_j \quad (10)$$

$$= \left(\frac{2}{a}\right)^N V_0 \cdot \frac{a}{2} \cdot \frac{a}{4} \cdot \left(\frac{a}{4}\right)^{N-2} = \frac{V_0}{2^{N-1}} \quad (11)$$

While the off-diagonal elements are calculated as follows:

$$\begin{aligned} W_{1i} &= \langle \psi_1 | H' | \psi_i \rangle \\ &= \left(\frac{2}{a}\right)^N V_0 \int_0^{a/2} \text{Sin}\left(\frac{\pi x_i}{a}\right) \text{Sin}\left(\frac{2\pi x_i}{a}\right) dx_i \int_0^a \text{Sin}\left(\frac{2\pi x_N}{a}\right) \text{Sin}\left(\frac{\pi x_N}{a}\right) dx_N \prod_{j=1}^{N-2} \int_0^{a/2} \text{Sin}^2\left(\frac{\pi x_j}{a}\right) dx_j \end{aligned}$$

Since the x_N integral in the above equation vanishes, we have

$$W_{1i} = W_{i1} = 0. \quad (12)$$

The other off-diagonal elements are

$$\begin{aligned} W_{ij} &= \langle \psi_i | H' | \psi_j \rangle \\ &= \left(\frac{2}{a}\right)^N V_0 \prod_0^{N-i} \int_0^{a/2} \text{sin}^2\left(\frac{\pi x}{a}\right) dx \int_0^{a/2} \text{Sin}\left(\frac{2\pi x_i}{a}\right) \text{Sin}\left(\frac{\pi x_i}{a}\right) dx_i \int_0^a \text{sin}\left(\frac{\pi x_j}{a}\right) \text{Sin}\left(\frac{2\pi x_j}{a}\right) dx_j \otimes \\ &\quad \int_0^a \text{Sin}^2\left(\frac{\pi x_N}{a}\right) dx_N \prod_0^{i-3} \int_0^{a/2} \text{Sin}^2\left(\frac{\pi x}{a}\right) dx \\ &= \left(\frac{2}{a}\right)^N V_0 \left(\frac{a}{4}\right)^{N-i} \left(\frac{2a}{3\pi}\right)^2 \cdot \frac{a}{2} \left(\frac{a}{4}\right)^{i-3} \\ &= \frac{V_0}{9\pi^2} \frac{1}{2^{N-7}} \end{aligned} \quad (13)$$

Equations (11) and (13) reduce to the three-dimensional values ($N=3$), namely, $(V_0 / 4)$ and

$(16V_0 / 9\pi^2)$ respectively (Griffiths, 1995). Defining $k \equiv \left(\frac{8}{3\pi}\right)^2$ and with the help of equations

(11), (12) and (13) we are able to construct the matrix W as

$$W = \frac{V_0}{2^{N-1}} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 1 & k & k & k & k & k & \dots & k \\ 0 & k & 1 & k & k & k & k & \dots & k \\ 0 & k & k & 1 & k & k & k & \dots & k \\ 0 & k & k & k & 1 & k & k & \dots & k \\ \cdot & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \cdot & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & k & k & k & k & k & k & \dots & 1 \end{pmatrix}_{(N \times N)}, \quad (14)$$

The eigen-values, λ are easier to find for the matrix $\frac{2^{N-1}}{V_0} W$ rather than W . This is achieved by setting

$$(1-\lambda) \begin{vmatrix} 1-\lambda & k & \dots & \dots & k \\ k & 1-\lambda & k & \dots & \dots & k \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ k & k & \dots & \dots & 1-\lambda \end{vmatrix}_{(N-1) \times (N-1)} = 0 \quad (15)$$

The characteristic equation of eq. (15) can be found by using (Hohn, 1973)

$$\det \begin{vmatrix} x+a & x & x & \dots & x \\ x & x+a & x & \dots & x \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ x & x & x & \dots & x+a \end{vmatrix}_{n \times n} = a^{n-1}(nx+a) \quad (16)$$

The identification $x \rightarrow k, a \rightarrow 1-\lambda-k$ and $n \rightarrow N-1$, yields the characteristic equation for eq. (15), with the result

$$(1-\lambda)(1-\lambda-k)^{N-2}[(N-1)k+(1-\lambda-k)] = 0 \quad (17)$$

The roots of the above equation are

$\lambda_1 = 1, \lambda_2 = 1+k(N-2)$, and $\lambda_3 = 1-k$, with λ_3 being $(N-2)$ degenerate.

Therefore, the energies, to first order, of the three distinct energy levels are

$$E_1 = \begin{cases} E_1^0 + \frac{V_0}{2^{N-1}} \\ E_1^0 + (1+k(N-2))\frac{V_0}{2^{N-1}} \\ E_1^0 + (1-k)\frac{V_0}{2^{N-1}} \end{cases}, \quad (18)$$

where E_1^0 is the (common) unperturbed energy given by eq. (6). We note that the perturbation H' lifts partially the degeneracy N to $(N-2)$, and splits E_1^0 into three distinct energy levels. It is interesting to note that the amount of splitting decreases as the space dimension N increases and it vanishes in the infinite dimensional space ($N \rightarrow \infty$). This can

be easily checked by taking the limit of the second terms in eq. (18) as $N \rightarrow \infty$. This shows that V_0 becomes weaker and hence the amount of splitting becomes smaller as the space dimension gets higher.

Sudden approximation for β -decay in N dimensions

In order to investigate the effect of space dimension on the results of the sudden approximation method, we consider an N -dimensional tritium atom consists of a nucleus 3H (containing one proton and two neutrons) and an electron. It is an unstable nucleus, since by β emission it decays into the nucleus 3He (containing two protons and one neutron), an electron e^- and an antineutrino $\bar{\nu}$ via the reaction ${}^3H \rightarrow {}^3He + e^- + \bar{\nu}$. The purpose here is to investigate the influence of β decay on the atomic electron in N -dimensional space. We assume that initially the tritium atom is in the ground state. In β decay process, the emitted electron from the tritium nucleus has an energy which, in most cases, is of the order of several keV. Therefore, the velocity v of the emitted electron is usually much larger than the velocity $v_0 = \alpha c \approx c/137$. of the atomic electron in the ground state of tritium. Thus, if the a_0 denotes the first Bohr radius, the β -electron will traverse the atom in a time $\tau \cong a_0/v$, which is much less than the periodic time $T = 2\pi a_0/v_0$ of the circulating atomic electron. Therefore, when tritium nucleus 3H decays by beta emission into 3He , the nuclear charge 'seen' by the atomic changes instantaneously from ze to $z'e$, with $z = 1$ and $z' = 2$. For time $t < 0$, the initial 3H atom has the Hamiltonian

$$H = H_0 = -\frac{\hbar^2}{2m} \nabla^2 - \frac{ze^2}{4\pi\epsilon_0 r}, \quad (19)$$

and for $t > 0$, the final 3He atom has the Hamiltonian

$$H = H_1 = -\frac{\hbar^2}{2m} \nabla^2 - \frac{z'e^2}{4\pi\epsilon_0 r}. \quad (20)$$

The eigen functions of H_0 and H_1 are the hydrogenic wave functions corresponding to $z = 1$ and $z' = 2$ respectively. The tritium atom is initially in the ground state ($n = 1, \ell = 0, m = 0$) and thus the probability amplitude $d^{(1)}_{n'\ell'm'}$ of finding the atomic electron in a discrete eigenstate ($n'\ell'm'$) of the 3He hydrogenic Hamiltonian H_1 at $t > 0$ is

$$d^{(1)}_{n'\ell'm'} = \langle \psi^{z'}_{n'\ell'm'} | \psi_{100}^z \rangle. \quad (21)$$

The hydrogenic wave function is

$$\psi_{n\ell m}^z(\vec{r}) = R_{n\ell}^z(r) Y_{\ell m}(\theta, \varphi), \quad (22)$$

where $R_{n\ell}^z(r)$ are the normalized radial hydrogenic wave function in N dimensions and $Y_{\ell m}(\theta, \varphi)$ are the hyperspherical harmonics that form orthonormal set, namely

$$\int Y_{\ell'm'}^*(\Omega) Y_{\ell m}(\Omega) d\Omega = \delta_{\ell\ell'} \delta_{mm'}. \quad (23)$$

The substitution of eq.(22) into eq.(21) and the use of eq.(23) show that the only non-vanishing probability amplitudes $d^{(1)}_{n'\ell'm'}$ are those corresponding to s-states ($\ell' = m' = 0$), therefore

$$d^{(1)}_{n'00} = \int R_{n'0}^{z'=2}(r) R_{10}^{z=1} r^{N-1} dr. \quad (24)$$

The radial solutions are given by (AL-Jaber, 1998)

$$R_{n\ell}^z(r) = A_{n\ell} \exp(-\rho/2) \rho^\ell L_{(n+\ell+N-3)}^{(2\ell+N-2)}(\rho) \quad (25)$$

where $\rho = \frac{2z}{a[n+(N-3)/2]}r$, with $a = \frac{\hbar^2}{me^2}$, $L_q^p(\rho)$ are the associated Laguerre polynomials and the normalization constant $A_{n\ell}$ is given by

$$A_{n\ell} = \left[\left(\frac{2z}{a(n+(N-3)/2)} \right)^N \frac{(n-\ell-1)!}{2[n+(N-3)/2]\{(n+\ell+N-3)!\}^3} \right]^{\frac{1}{2}}. \quad (26)$$

For $n = 1$ and $\ell = 0$, eq.'s (25) and (26) become

$$R_{10}^z(r) = A_{10} \exp(-\rho/2) L_{(N-2)}^{(N-2)}(\rho) \quad (27)$$

$$A_{10} = \left[\left(\frac{4z}{a(N-1)} \right)^N \frac{1}{(N-1)[(N-2)!]^3} \right]^{\frac{1}{2}}, \quad (28)$$

with $\rho = \frac{4z}{a(N-1)}r$. Using $L_{(N-2)}^{(N-2)}(\rho) = 1$ and substituting eq.'s (27) and (28) into eq. (24),

we get

$$d_{100}^{(1)} = A_{10}^z A_{10}^{z'} \int_0^\infty \exp\left[-\frac{6r}{a(N-1)}\right] r^{N-1} dr. \quad (29)$$

Upon substituting $z = 1$ and $z' = 2$ in the constants A_{10}^z and $A_{10}^{z'}$ we get

$$A_{100}^1 A_{10}^2 = 2^{N/2} \left(\frac{4}{a(N-1)} \right)^N \frac{1}{(N-1)[(N-2)!]^3}, \quad (30)$$

and with the help of the formula

$$\int_0^\infty e^{-x} x^{N-1} dx = \Gamma(N), \quad (31)$$

the integral in eq. (29) yield $\left[\frac{a(N-1)}{6} \right]^N \Gamma(N)$, where $\Gamma(N)$ is the gamma function.

Therefore, eq. (29) becomes

$$\begin{aligned} d_{100}^{(1)} &= A_{10}^1 A_{10}^2 \left[\frac{a(N-1)}{6} \right]^N \Gamma(N) \\ &= \frac{2^{3N/2}}{3^N} \Gamma(N) \frac{1}{(N-1)[(N-2)!]^3}, \end{aligned}$$

which simplifies to

$$d_{100}^{(1)} = \frac{2^{3N/2}}{3^N} \frac{1}{[(N-2)!]^2}. \quad (32)$$

The above equation clearly shows the dependence of the probability amplitude on the space dimension N , and it reduces to its well-known value for the three-dimensional case (Bransden

and Joachain, 2000), namely $d_{100}^{(1)} = \frac{16\sqrt{2}}{27}$ for $N=3$.

The probability, $P_{100}^{(1)}$ that the (${}^3\text{He} + \bar{e}$) ion be found in its ground state is

$$P_{100}^{(1)} = |d_{100}^{(1)}|^2 = \left(\frac{8}{9}\right)^N \frac{1}{[(N-2)!]^4}, \quad (33)$$

which gives the expected result [42], $P_{100}^{(1)} = \frac{512}{729}$ for $N=3$. The total probability for excitation and ionization of the (${}^3\text{He} + \bar{e}$) ion is therefore

$$P_{total} = (1 - P_{100}^{(1)}) = 1 - \left[\left(\frac{8}{9}\right)^N \frac{1}{[(N-2)!]^4} \right]. \quad (34)$$

Eq.'s (33) and (34) clearly show that as the space dimension N increases $P_{100}^{(1)}$ (P_{total}) decreases (increases), and if $N \rightarrow \infty$, then $P_{100}^{(1)}$ (P_{total}) $\rightarrow 0$ (1). This means that when tritium atom undergoes a β -decay, the higher the space dimension the higher the probability of excitation and ionization of (${}^3\text{He} + \bar{e}$) ion and the lower to be in the ground state.

CONCLUSIONS AND RESULTS

In the present paper, the role of the space dimension N on the results obtained by approximation methods has been investigated. This gives an opportunity for involving students in an in-depth study of quantum systems in higher space dimensions, To that end, two approximation methods were applied to quantum systems in N -dimensional space. In the first method, degenerate perturbation theory was employed for a perturbed N -dimensional infinite cubical well. It was found that the perturbation H' lifts partially the degeneracy N , of the unperturbed system, to $(N-2)$. It was also observed that the perturbation splits the unperturbed energy E_1^0 , into three distinct energy levels with one of them being $(N-2)$ degenerate. It is remarkable to notice that the amount of energy difference for splitting decreases as the space dimension increases and it vanishes in the infinite dimensional space. The decrease of the matrix elements with N seems to be due to the multiplicative effect of factors smaller than 1, the number of which increases with N . In the second method, the sudden approximation method was applied to the process of β -decay of tritium atom in N dimensions. Assuming that the tritium atom is initially in the ground state, it was found that the probability that the (${}^3\text{He} + \bar{e}$) ion to be in the ground state depends on the space dimension N . In addition, this probability decreases as N increases and it vanishes as $N \rightarrow \infty$. This means that the total probability of excitation and ionization increases as N increases and approaches unity in the infinite dimensional space. One may argue that the results come from the fact that as N increases, the eigenvalues of the attractive $1/r$ potential get closer to zero. Thus, the ionization becomes easier, and it becomes even a spontaneous transition in the limit of infinite N .

Therefore, our results clearly show the effect of the space dimension on the results predicted by approximation methods when applied to quantum systems.

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بعض الملاحظات على طرق تقريب لأنظمة كمية في أبعاد فضائية عالية

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الملخص

نعرض تأثير البعد الفضائي N على النتائج المتوقعة من تطبيق طريقتي تقريب على أنظمة فيزيائية كمية. في التقريب الأول، سنطبق نظرية الاضطراب الانحلالي على تجويف مكعب لانهائي مضطرب في بعد فضائي N . لقد وجد أن فرق الطاقة للانقسام يتناقص عندما تتزايد قيمة N ويتلاشى هذا الفرق في بعد فضائي لانهائي. في التقريب الثاني، سنطبق طريقة التقريب المفاجئ على اضمحلال بيتا لنواة التريتيوم في أبعاد عالية. وجد أنه كلما زادت قيمة N فإن احتمال الاضمحلال يتناقص وبالتالي فإن احتمال التآين يتزايد.