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Nonstructural theory of the exciton states in solid rare gases

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We develop a simple nonstructural theory of the exciton states in solid rare gases. The potential energy in the Schrödinger equation of the free rare-gas atom is parametrized in the simplest form which reproduces the exact experimental excited atomic levels. The same equation is modified to describe the exciton states in the solid phase simply by introducing the effective mass μ and by screening the Coulomb potential outside the atom with the dielectric constant ϵ_0 of the solid. In this way the exciton levels in the effective-mass approximation become continuously the excited atomic levels, as the effective Rydberg approaches the Rydberg constant. This solves the dilemma between the Wannier and the Frenkel models for all spectroscopic terms, i.e., for the high as well as for the low exciton levels. It also solves the problem for the whole series of solid rare gases, in which quite different values of μ and ϵ_0 occur. Complete agreement is achieved in the comparison of the theoretical results with the experimental data. Accurate values are also obtained for μ and for the energy gaps E_g^s; they differ substantially from those generally accepted within the framework of the Wannier model. The exchange and spin-orbit interactions are shown to be identical in the solid phases and in the free atoms.

I. INTRODUCTION

The study of the electronic states in solid rare gases is of great importance in solid-state physics. Rare-gas atoms are closed-shell systems; the interactions among them in the solid phase are due to weak van der Waals forces. Then, as in other more complex molecular crystals, many characteristics of the free constituent elements are preserved. The optical-absorption edges for electronic transitions exhibit a large number of exciton peaks; this has been a puzzle for a considerable time. There is, in fact, a dilemma between an atomic-type classification of the levels and the Wannier model. It is observed that the higher members of the series, characterized by principal quantum numbers $n \geqslant 2$, fit well within the Wannier model, whereas the lowest exciton states, with $n = 1$, do not. It is also observed that this discrepancy is very large in solid neon, of the order of 1 eV, and that it gradually disappears as we proceed down the appropriate column in the Periodic Table. These discrepancies are approximately 0.2, 0.06, and 0.00 eV in solid argon, krypton, and xenon, respectively.

The effective masses μ and the energy gaps E_g^s have been obtained from the Wannier model fitted to the series higher terms ($n \geqslant 2$). The binding energies of the lowest levels ($n = 1$) have been specified in reference to those energy gaps E_g^s and have been calculated within several models by introducing atomic-type central-cell corrections.[1-4] However, these theories are all based on the band structure of the crystal. Such a structure does not exist for the free atom, and the corresponding energies and wave functions are not suitable to establish a direct relationship with the excited atomic levels.

Recently it has been pointed out that the band structure of the solid is not essential for the determination of the positions of the exciton levels and that a nonstructural approach which works in direct space is more appropriate.[5-7] We have shown that approximate solutions which have the proper behavior in both the effective-mass approximation (EMA) and the atomic limit provide the correct trend of the exciton levels throughout the solid-rare-gas series.[6] Furthermore, a calculation which fully exploits the atomic limit shows that a quantum-defect classification must replace the Wannier model in solid neon.[7] It is possible to develop a quantum-defect theory for the solid phase with the condition of correct behavior of the solutions in both the EMA and the atomic limit. Such a theory can simply explain all exciton levels in the whole solid-rare-gas series. We proceed as follows.

The EMA is simply the Schrödinger equation for the hydrogen atom with two oppositely charged particles of reduced mass μ interacting through a Coulomb potential screened by the static dielectric constant ϵ_0 of the solid. If we let ϵ_0 and μ (in electron mass units) approach unity, the EMA yields the hydrogen atom levels. The rare-gas atomic levels are quite different from these so that our model should give the latter as ϵ_0 and μ approach unity. On the other hand, the EMA limit must hold when the effective Rydberg becomes small compared to the Rydberg constant, since the excitations become much more extended in the solid than in the free atom. To obtain both results, we have simply to cut off the screened Coulomb potential inside the atom in the EMA equation and replace it in such a way as to obtain the rare-gas atomic levels for $\epsilon_0 = \mu = 1$. In this fashion, the atomic and the EMA limits transform continuously into one another with varying ϵ_0 and μ. The necessity to distinguish between $n \geq 2$ and $n = 1$ states in the Wannier and in the Frenkel models disappears: a single generalization of both models applies to all levels. We can also determine accurate values for μ and E_g^s. These values differ from those provided by the Wannier model as we move towards the atomic limit; they approach them in the EMA limit. Solid neon turns out to be close to the atomic limit, whereas solid xenon is essentially described by the EMA. Solid argon and krypton are intermediate, and the theory provides an accurate description for all four solid rare gases considered. The details are described in Sec. II. A preliminary account of the results has been given elsewhere.[8]

II. NONSTRUCTURAL APPROACH

We set up the Schrödinger equations

$$-\tfrac{1}{2}\chi_n^{a\prime\prime} + U_n^a(r)\chi_n^a = -W_n^a\chi_n^a \qquad (1)$$

and

$$-(1/2\mu)\chi_n^{s\prime\prime} + U_n^s(r)\chi_n^s = -W_n^s\chi_n^s , \qquad (2)$$

for the s-type envelope functions χ_n^a and χ_n^s of the free atom and the solid excitations, respectively. Equations (1) and (2) are written in atomic units, $n = 1, 2, \ldots,$ and W_n^a and W_n^s are the binding energies of the excited states in the free atom and in the solid phase, respectively. W_n^a and W_n^s are related to the corresponding excitation energies E_n^a and E_n^s through the equations

$$W_n^a = E_g^a - E_n^a \qquad (3)$$

and

$$W_n^s = E_g^s - E_n^s . \qquad (4)$$

E_g^a and E_g^s are series limits, i.e., the ionization potential in the free atom and the interband energy gap in the solid phase, respectively. The potential energies in Eqs. (1) and (2) are

$$U_n^a(r) = -r^{-1} , \qquad (5)$$

$$U_n^s(r) = -(\epsilon_0 r)^{-1} \qquad (6)$$

outside the atomic radius ρ_a, defined as half of the nearest-neighbor distance in the solid,[9] and

$$U_n^a(r) = U_n^s(r) = -C_n \qquad (7)$$

inside the atomic radius ρ_a. The constants C_n must be such that the eigenvalues W_n^a of the atomic Eq. (1) are the exact experimental excitation energies of the free atom.[10] Since ρ_a is not small compared to 1 a.u., Eq. (1) is, of course, not the hydrogen atom equation, but a model equation for the excited states of the rare-gas atom we are considering. Equation (2) is identical to it for $\mu = \epsilon_0 = 1$ (atomic limit), but its solutions approach the EMA solutions when the effective Rydberg R^s,

$$R^s = \mu/2\epsilon_0^2 , \qquad (8)$$

becomes small compared to the Rydberg constant $R = 0.5$ a.u. $= 13.606$ eV of the hydrogen atom (EMA limit).

One can think at first sight that Eqs. (1)–(7) are too simple to describe the problem. We believe, however, that they contain the essential physics. Let us consider first the free atom. It is known that the many-body problem of the atomic excitations can be reduced to a two-body problem in the framework of the quantum-defect theory.[11] This theory is based on the fact that a Schrödinger equation for a two-particle pseudoeigenfunction can be derived, and that the pseudopotential involved is Coulombic for large r and finite in the atomic region. If we write the excitation binding energies as

$$W_n^a = R(n + \delta_n^a)^{-2} , \qquad (9)$$

with $n = 1, 2, \ldots,$ such hypotheses on the potential lead to the fact that the quantum defects δ_n^a are fairly constant as functions of n and generally smaller than unity. This result is experimentally verified for all atoms. If we consider, for instance, the neon and xenon atoms, the valence excitations can be pictured as promotions of an electron from the $2p$ and $5p$ orbitals to $(n+2)s$ and $(n+5)s$ orbitals, respectively. Despite the remarkable differences in size, in number of electrons, and in nodal structure and extension of the orbitals, the experimental quantum defects δ_n^a do not differ by much (see Table I). Therefore, within the point of view of the quantum-defect theory, Eqs. (1), (5) and (7) are justified. We note that the Coulomb potential of Eq. (5) is appropriate outside the atomic radius ρ_a, whereas the choice of Eq. (7) inside ρ_a is dictated only by simplicity. In fact, the true potential in this region is an unknown complicated state-dependent function.[12] Since we are not interested in solving *a priori* the atomic problem, our choice provides the exact experimental atomic limit in the simplest way. The choice of constant potential in the atomic region is commonly made in quantum-defect calculations. Equations (1), (5), and (7) constitute the problem of the Coulomb potential with cutoff. A recent example of such a study is that of Linz and Chen,[13] who have carried out a calculation of the exact eigenvalues W_n^a of these equations requiring the potential to be continuous, i.e., setting

TABLE I. Experimental transition energies E_n^a, quantum defects δ_n^a, ionization potentials E_g^a of rare-gas atoms. Data from Ref. 10. Energies are in eV.

	Neon				Argon			
J	$\frac{3}{2}$		$\frac{1}{2}$		$\frac{3}{2}$		$\frac{1}{2}$	
	E_n^a	δ_n^a	E_n^a	δ_n^a	E_n^a	δ_n^a	E_n^a	δ_n^a
$n = 1$	16.668	0.6676	16.846	0.6814	11.622	0.8139	11.826	0.8198
2	19.685	0.6930	19.777	0.6893	14.088	0.8549	14.253	0.8444
3	20.568	0.7001	20.660	0.6916	14.846	0.8644	15.020	0.8565
4	20.946	0.7030	21.040	0.6934	15.183	0.8686	15.357	0.8537
5	21.143	0.7047	21.238	0.6932	15.364	0.8805		
6	21.259	0.7050						
E_g^a	21.561		21.658		15.757		15.935	

	Krypton				Xenon			
J	$\frac{3}{2}$		$\frac{1}{2}$		$\frac{3}{2}$		$\frac{1}{2}$	
	E_n^a	δ_n^a	E_n^a	δ_n^a	E_n^a	δ_n^a	E_n^a	δ_n^a
$n = 1$	10.031	0.8521	10.642	0.8395	8.435	0.9195	9.568	0.8760
2	12.383	0.9034	13.035	0.8904	10.592	0.9759	11.876	0.9549
3	13.112	0.9197	13.761	0.8826	11.272	0.9879		
4	13.435	0.9162	14.096	0.8987	11.581	0.9878		
5	13.609	0.9169	14.272					
E_g^a	13.997		14.663		12.128		13.434	

$$C_n = \rho_a^{-1} \tag{10}$$

for $r \leq \rho_a$.

Since the quantum defects δ_n^a are rather constant and usually smaller than unit, their effects upon Eq. (9) quickly disappear with increasing n, and the Rydberg series

$$W_n^a = Rn^{-2} \tag{11}$$

is obtained. Similarly, the Wannier series,

$$W_n^s = R^s n^{-2} \tag{12}$$

are observed in the solid phases for $n \geq 2$. However, these also must be considered approximations of the quantum-defect series,

$$W_n^s = R^s(n + \delta_n^s)^{-2}, \tag{13}$$

which hold for all n. It has been shown[7] in the case of solid neon that a quantum-defect fitting of all levels leads to an effective Rydberg R^s and a series limit E_g^s different from those generally accepted according to the Wannier-model fit of the $n \geq 2$ levels.

Consider now Eqs. (2), (6), and (7) for the solid phase. The transformation of the many-body problem to a two-body problem can be accomplished quite straightforwardly in the envelope-function theory.[6,14] We have used its language for both the solid phase and the free atom. We could, however, equally well, have used the language of the pseudopotential theory. We remark, in particular, that pseudopotentials of the type given in Eqs. (6) and (7) have been successfully used by many workers in solid-state physics and are referred to as Heine-Abarenkov model potentials.[15]

Equations (1), (2), (5), (6), and (7) establish a procedure to calculate the excitation binding energies W_n^s in the solid phase exactly. The method of solution is the following. Equations (1) and (5) are solved numerically for $r \geq \rho_a$ for any given exact experimental excitation binding energy W_n^a of the free atom.[10] The condition of regularity at infinity,

$$\chi_n^a(r) \xrightarrow[r\to\infty]{} 0, \tag{14}$$

determines a unique outer logarithmic derivative

$$D_{n,\mathrm{out}}^a(r) = \chi_n^{a\prime}(r)/\chi_n^a(r). \tag{15}$$

Equations (1) and (7) are solved analytically for $r \leq \rho_a$. The inner logarithmic derivative of the function, regular at the origin, is

$$D_{n,\mathrm{in}}^a(r, C_n) = k \cot kr, \tag{16}$$

where

$$k = [2(C_n - W_n^a)]^{1/2}. \tag{17}$$

$D_{n,\mathrm{in}}^a(\rho_a, C_n)$ is a monotonically decreasing function of C_n in the interval $0 \leq k\rho_a$ and varies within the interval $[\rho_a^{-1}, -\infty]$. By matching this quantity with $D^a_{n,\,\mathrm{out}}(\rho_a)$, a unique value for C_n is determined.

In the solid phase, we look for the solutions $\chi^s(r,W^s)$ of the equation

$$-(1/2\mu)\chi^{s\prime\prime}+U^s_n(r)\chi^s=-W^s\chi^s\,, \qquad (2')$$

regular at infinity and at the origin. The potential is given by Eqs. (6) and (7) and W^s ranges from C_n to zero. The difference between the outer and inner logarithmic derivatives at $r=\rho_a$ exhibits a series of zeros and poles as a function of W^s. The nth zero is the eigenvalue W^s_n we look for. In order to determine it, several numerical integrations of Eqs. (2′) and (6) for different W^s must be performed. Tests on the whole structure of zeros and poles are necessary. We have developed a program in interactive FORTRAN which solves the problem accurately. The input are the quantities $W^a_n, \rho_a, \epsilon_0$, and μ, and the output are C_n and W^s_n.

In order to obtain theoretical results which can be compared to the experimental data we need to know the dielectric constant ϵ_0 and the effective mass μ. However, while ϵ_0 is measured directly, μ is not. The accepted "experimental" value of μ is obtained by fitting the experimental energy levels with $n\geq 2$ with the Wannier model [Eq. (12)]. We have already discussed why this is not appropriate. On the other hand, several different energy-band calculations[16] have provided sets of values for μ. In contrast with previous theories we do not select any *a priori* value. We use μ as a parameter which we fit to the experimental data.

The data yield values for the transition energies E^s_n, whereas the theoretical calculations provide binding energies W^s_n. In order to make a comparison, knowledge of the energy gaps E^s_g is required. These quantities are not measured directly, and again their accepted "experimental" values originate from a fit of the Wannier model to the data $E^{s(\mathrm{expt})}_n$ for $n\geq 2$. On the other hand, the values of E^s_g given by energy-band calculations range over several eV. Therefore, the energy gaps E^s_g are practically unknown. We determine them independently, by comparing the calculated energy differences $W^s_n - W^s_{n+1}$ with the experimental differences $E^{s(\mathrm{expt})}_n - E^{s(\mathrm{expt})}_{n+1}$ adjusting the value of μ. This provides agreement with the experimental data for all levels within their accuracy of the order of 0.01 eV.[17] Therefore, to the same accuracy, E^s_g is obtained by adding W^s_n and $E^{s(\mathrm{expt})}_n$. We shall see later how our values of μ and E^s_g compare with those given by previous studies. For the moment, we point out that this theory involves considerably fewer parameters than the data it describes and that it is self-consistent.

Finally we mention that for each n there are, in fact, four spin-orbit split components, two of which, denoted by $\frac{3}{2}$ and $\frac{1}{2}$, are optically allowed.[18] In the present theory, the short-range exchange and spin-orbit interactions in the solid phase are included in the constants C_n determined from the free atom data, so that each component can be considered independently.[6] The comparison with the experimental data confirms the validity of this assumption.

III. RESULTS OF THE CALCULATION

Table I displays the lower experimental transition energies E^a_n, series limits E^a_g, and quantum defects δ^a_n of the rare-gas atoms.[10] The data and the significant figures we keep are those needed for our purposes. In Table II we give the corresponding theoretical quantities E^s_n, E^s_g, and δ^s_n for the solid phases, obtained by solving Eqs. (1)–(7), and the values of the effective masses μ and effective Rydbergs R^s. For comparison in Table III we exhibit the experimental data[17] $E^{s(\mathrm{expt.})}_n$ for the transition energies of solid rare gases. The values of the dielectric constants ϵ_0 and of the atomic radii ρ_a used in the calculation are given in Table IV. The references from which these data are taken are quoted in Ref. 6.

We note that in solid neon R^s is comparable to $R=13.606$ eV, and accordingly δ^s_n and E^s_g turn out close to δ^a_n and E^a_g for the free atom. In solid xenon, where R^s is about 15 times smaller than R, δ^s_n becomes ten times smaller than δ^a_n, and it is almost negligible compared to n. Also, E^s_g is about 3 eV lower than E^a_g. It is clear that, while neon is close to the atomic limit, solid xenon approximates the EMA limit. The cases of solid argon and krypton are intermediate. It is very satisfactory to find that this type of nonstructural approach describes all situations so simply and effectively.

We note that the energy gaps E^s_g and the effective masses μ inferred from fitting of the Wannier model to the experimental data $E^{s(\mathrm{expt})}_n$ for $n\geq 2$ are $E^s_g=21.49$ eV, 14.14 eV, 11.61 eV, 9.31 eV, and $\mu=0.56$, 0.46, 0.39, 0.34 in solid neon, argon, krypton, and xenon, respectively for the $\frac{3}{2}$ series. We see from Table II that these assignments are not appropriate in the case of solid neon, while they become gradually correct as we move toward solid xenon.

The range of values of the results of energy-band calculations[16] are $E^s_g=22.16$–25.5 eV, 7.60–18.52 eV, 11.30–16.46 eV, 7.87 eV, and $\mu=0.78$, 0.44–0.45, 0.36–0.49, 0.30–0.40, in solid neon, argon, krypton, and xenon, respectively. It is well known that the energy-band calculations cannot usually provide reliable values for the energy gaps E^s_g. The fact that the values of μ obtained here and

TABLE II. Theoretical transition energies E_n^s, quantum defects δ_n^s, energy gaps E_g^s, effective Rydbergs R^s, and masses μ of solid rare gases. Energies are in eV; effective masses in electron mass units.

	Neon				Argon			
J	$\frac{3}{2}$		$\frac{1}{2}$		$\frac{3}{2}$		$\frac{1}{2}$	
	E_n^s	δ_n^s	E_n^s	δ_n^s	E_n^s	δ_n^s	E_n^s	δ_n^s
$n = 1$	17.58	0.4597	17.79	0.4761	12.04	0.1994	12.25	0.2060
2	20.24	0.5009	20.35	0.4967	13.57	0.2675	13.75	0.2576
3	20.91	0.5129	21.03	0.5039	13.89	0.2854	14.07	0.2783
4	21.19	0.5182	21.31	0.5080	14.00	0.2934	14.18	0.2803
5	21.33	0.5211	21.45	0.5090	14.06	0.3061		
6	21.41	0.5239						
E_g^s	21.61		21.73		14.17		14.35	
R^s	8.58,	$\mu = 0.97$	8.58,	$\mu = 0.97$	3.06,	$\mu = 0.62$	3.06,	$\mu = 0.62$

	Krypton				Xenon			
J	$\frac{3}{2}$		$\frac{1}{2}$		$\frac{3}{2}$		$\frac{1}{2}$	
	E_n^s	δ_n^s	E_n^s	δ_n^s	E_n^s	δ_n^s	E_n^s	δ_n^s
$n = 1$	10.17	0.0761	10.86	0.0734	8.37	0.0078	9.51	-0.0280
2	11.24	0.1452	11.93	0.1411	9.08	0.0770	10.29	0.0630
3	11.44	0.1659	12.13	0.1614	9.20	0.0937		
4	11.50	0.1675	12.30	0.1630	9.24	0.0979		
5	11.54	0.1704						
E_g^s	11.60		12.29		9.30		10.51	
R^s	1.65,	$\mu = 0.43$	1.61,	$\mu = 0.42$	0.94,	$\mu = 0.34$	0.94,	$\mu = 0.34$

those found in the band-structure studies differ in solid neon and argon is not a contradiction. The band-structure results refer to the center of the Brillouin zone, whereas those in the present work represent averages over the whole zone, because all $\vec{k}$ states are necessary for the formation of localized excitons.[4,6] Note, however, that in the exact atomic limit (atoms far apart) the correct value must be $\mu = 1$ in both cases. The same value of μ must be found in the exact EMA limit as well. The values given by the present work lie within the range of those provided by the band-structure calculations in solid krypton and xenon.

We note finally that the splittings $W_n^s(\frac{1}{2}) - W_n^s(\frac{3}{2})$ and $E_g^s(\frac{1}{2}) - E_g^s(\frac{3}{2})$ between the components of the levels belonging to the $\frac{1}{2}$ and $\frac{3}{2}$ series are equal to the corresponding values in the free atoms within a few hundredths of an eV. This agrees with the experimental situation.

TABLE III. Experimental transition energies $E_n^{s(\mathrm{expt})}$ of solid rare gases in eV. Data from Ref. 17.

J	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{1}{2}$
	Neon		Argon	
$n = 1$	17.59	17.79	12.06	12.24
2	20.25	20.37	13.57	13.75
3	20.92	21.02	13.89	14.07
4	21.18	21.24?	13.97	
5	21.29			
	Krypton		Xenon	
$n = 1$	10.17	10.86	8.37	9.51
2	11.23	11.92	9.07	
3	11.44	12.21?	9.21	
4	11.52			

TABLE IV. Dielectric constants ϵ_0 and atomic radii ρ_a in a.u. The experimental references are quoted in Ref. 6.

	Ne	Ar	Kr	Xe
ϵ_0	1.24	1.660	1.882	2.217
ρ_a	2.96	3.545	3.777	4.101

The values obtained for the effective masses μ are very close for both the $\frac{3}{2}$ and $\frac{1}{2}$ series. In the case of solid xenon, since there is only one experimentally available value $E_1^{s(\mathrm{expt})}(\frac{1}{2})$ for the $\frac{1}{2}$ series, $\mu(\frac{1}{2})$ and $E_g^s(\frac{1}{2})$ cannot be determined independently. The assumption of Table II is to set $\mu(\frac{1}{2}) = \mu(\frac{3}{2})$ in solid xenon. Another assumption would be to set $E_g^s(\frac{1}{2}) - E_g^s(\frac{3}{2}) = E_g^a(\frac{1}{2}) - E_g^a(\frac{3}{2})$ which would lead to the values $E_g^s(\frac{1}{2}) = 10.61$ eV, $\mu(\frac{1}{2}) = 0.38$, and $E_1^s(\frac{1}{2}) = 9.50$ eV. The truth must be between these two descriptions.

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