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Energy bands and excitons in solid neon

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The energy bands of solid neon are computed with a modified orthogonalized plane-wave method, which includes rigorously the Hartree-Fock exchange potential in its nonlocal form. Starting from the computed energy bands, the binding energies for valence and core excitons are obtained. The results are compared with earlier calculations and with experiments.

I. INTRODUCTION

Energy bands and excitons in neon have been investigated both experimentally and theoretically by a large number of authors.[1,2] The band structure of neon has been computed with the Korringa-Kohn-Rostoker (KKR) method,[3] the augmented-plane-wave (APW) method[4], also using electron-atom scattering phase shifts,[5] and the localized orbital method with Slater-type orbitals (STO's) (Ref. 6) or Gaussian-type orbitals (GTO's).[7] For a thorough comparison of the results of the various methods we refer to the discussion of Rossler.[1] Here we only mention that the major source of inaccuracy and discrepancy seems to be related to the difficult task of the evaluation of the exchange term in its nonlocal form. In the case of argon, for instance, Lipari and Fowler[8] have shown that the orthogonalized plane-wave (OPW) method with nonlocal exchange gives the acceptable Hartree-Fock (HF) energy gap of ≈ 17 eV, while the often adopted local Slater approximation [Hartree-Fock-Slater (HFS)] would lead to ≈ 7 eV. In the case of LiH, it has been shown[9] that the HF energy gap is ≈ 9 eV, while the HFS approximation fails to reproduce the insulating character of this compound.

In Sec. II, we compute the band structure of neon using the OPW method with the exchange potential in its nonlocal form. The computational method used is an extention of the new procedure recently tested in the case of solid lithium hydride[9]; the exchange integrals involving two plane waves and two localized functions are evaluated analytically through the Dawson auxiliary function, thus drastically reducing the amount of computational labor.

In Sec. III we calculate the binding energies of valence and core excitons. Following the most recent developments on exciton theory (see, for instance, Refs. 10–14 and references quoted therein), the crucial problem of central cell corrections is solved exploiting the accurately known experimental energies of excitons in the isolated neon atom. The band kinetic operator, corresponding to our computed energy bands, is treated with an appropriate variational method. Section IV contains the conclusions.

II. ENERGY BANDS OF NEON BY THE OPW METHOD

A. Details of calculation

The computational method used in the present work is an extension of the procedure recently put forward in the case of lithium hydride.[9] Here we briefly summarize some relevant aspects, sending the reader for more details to Ref. 9.

The crystal structure of solid neon is fcc, with lattice parameter $a = 8.43$ a.u. The fundamental vectors of the direct (reciprocal) lattice are given by

$$\vec{\tau}_1 = \tfrac{1}{2}a(0,1,1) \quad [\vec{h}_1 = (2\pi/a)(-1,1,1)]$$

and cyclic permutations.

The neon atom has the closed-shell electronic configuration $1s^2$, $2s^2$, $2p^6$. In the minimal basis set, the optimized screenings[15] of $1s$, $2s$, and $2p$ Slater-type orbitals are $\xi_{1s} = 9.6421$ a.u., $\xi_{2s} = \xi_{2p} = 2.8792$. The ionization energies are taken as $E_{1s} = -62.99$ (Ref. 16), $E_{2s} = -3.568$ (Ref. 17), and $E_{2p} = -1.585$ Ry (Ref. 18). To set up the OPW method for describing the conduction energy bands, we orthogonalize plane waves to the five Bloch sums corresponding to $1s$, $2s$, $2p_x$, $2p_y$, and $2p_z$ wave functions of neon.

All the matrix elements appearing in the OPW method, including the exchange potential in its nonlocal form, can be evaluated analytically (see Ref. 9 and references quoted therein). The explicit expression of the OPW matrix elements is reported in Ref. 9 in the case where the occupied states are s like; here we give the extensions appropriate for p like occupied states.

In the OPW method the exact account of the exchange potential in its nonlocal form requires the evaluation of bielectronic integrals involving two plane waves and two Slater-type localized functions. The first step toward an accurate and simple numerical evaluation consists in expanding STO's into GTO's. The expansion is performed using the scaling theorem and the universal parameters available in the literature (see, for instance, Ref. 19). For instance, the parameters for the 4G representation of 1s, 2s, and 2p orbitals of neon, obtained by the least-squares method,[19] are reported in Table I.

Next, we have to evaluate the fundamental integrals:

$$J_s(\vec{K}_i,\alpha,\beta,\vec{K}_j)=\int e^{-i\vec{K}_i\cdot\vec{r}_1}e^{-\alpha r_2^2}Y_{00}^*(\vec{r}_2)\frac{1}{|\vec{r}_1-\vec{r}_2|}\times e^{-\beta r_1^2}Y_{00}(\vec{r}_1)e^{i\vec{K}_j\cdot\vec{r}_2}d\vec{r}_1\,d\vec{r}_2 \qquad (1)$$

$$J_p(\vec{K}_i,\alpha,\beta,\vec{K}_i)=\sum_{m=-1,0,1}\int e^{-i\vec{K}_i\cdot\vec{r}_1}r_2\,e^{-\alpha r_2^2}Y_{1m}^*(\vec{r}_2)\frac{1}{|\vec{r}_1-\vec{r}_2|}\times r_1e^{-\beta r_1^2}Y_{1m}(\vec{r}_1)e^{i\vec{K}_j\cdot\vec{r}_2}d\vec{r}_1\,d\vec{r}_2\ . \qquad (2)$$

Expression (1) has been given in Ref. 9 in terms of the auxiliary Dawson function[20]

$$\Phi(x)=\frac{1}{x}e^{-x^2}\int_0^x e^{t^2}\,dt\ . \qquad (3)$$

We have

$$J_s(\vec{K}_i,\alpha,\beta,\vec{K}_j)=\frac{\pi^{3/2}}{2\alpha\beta(\alpha+\beta)^{1/2}}\exp\left(-\frac{(\vec{K}_i-\vec{K}_j)^2}{4(\alpha+\beta)}\right)\Phi(K\sqrt{\gamma}), \qquad (4)$$

where

$$\gamma=\frac{\alpha\beta}{\alpha+\beta}\ ,\quad \vec{K}=\frac{1}{2}\left(\frac{\vec{K}_i}{\beta}+\frac{\vec{K}_j}{\alpha}\right)\ .$$

To evaluate expression (2) we use the addition theorem for spherical harmonics and we obtain

$$J_p(\vec{K}_i,\alpha,\beta,\vec{K}_j)=\frac{3}{4\pi}\int\vec{r}_1\cdot\vec{r}_2\,e^{-i\vec{K}_i\cdot\vec{r}_1}e^{-\alpha r_2^2}\times\frac{1}{|\vec{r}_1-\vec{r}_2|}e^{-\beta r_1^2}e^{i\vec{K}_j\cdot\vec{r}_2}d\vec{r}_1\,d\vec{r}_2$$

$$=3\sum_{l=x,y,z}\frac{\partial}{\partial K_{il}}\frac{\partial}{\partial K_{jl}}J_s(\vec{K}_i,\alpha,\beta,\vec{K}_j)\ . \qquad (5)$$

We put Eq. (4) into Eq. (5) and we notice that any derivative of the Dawson function (3) can be expressed in terms of the Dawson function itself. With somewhat lengthy but straightforward algebra we have

TABLE I. Parameters for the 4G representation of 1s, 2s, and 2p Slater-type orbitals. The values α_i and c_i are taken from Ref. 19.

$\psi_{1s}(\vec{r})=2\xi^{3/2}e^{-\xi r}Y_{00}(\vec{r})$	
$\approx\frac{2^{7/4}}{\pi^{1/4}}\left(\sum_{i=1}^{4}c_i(\alpha_i\xi^2)^{3/4}e^{-\alpha_i\xi^2r^2}\right)Y_{00}(\vec{r})$	
α_i	c_i
8.80187×10^{-2}	2.91626×10^{-1}
2.65204×10^{-1}	5.32846×10^{-1}
9.54620×10^{-1}	2.60141×10^{-1}
5.21686	5.67523×10^{-2}
$\psi_{2s}(\vec{r})=\frac{2}{\sqrt{3}}\xi^{5/2}re^{-\xi r}Y_{00}(\vec{r})$	
$\approx\frac{2^{7/4}}{\pi^{1/4}}\left(\sum_{i=1}^{4}c_i(\alpha_i\xi^2)^{3/4}e^{-\alpha_i\xi^2r^2}\right)Y_{00}(\vec{r})$	
α_i	c_i
6.28104×10^{-2}	4.97767×10^{-1}
1.63541×10^{-1}	5.58855×10^{-1}
5.02989×10^{-1}	2.97680×10^{-5}
2.32350	-6.22071×10^{-2}
$\psi_{2pm}(\vec{r})=\frac{2}{\sqrt{3}}\xi^{5/2}re^{-\xi r}Y_{1m}(\vec{r})$	
$\approx\frac{2^{11/4}}{\sqrt{3}\pi^{1/4}}\left(\sum_{i=1}^{4}c_i(\alpha_i\xi^2)^{5/4}re^{-\alpha_i\xi^2r^2}\right)Y_{1m}(\vec{r})$	
α_i	c_i
6.28104×10^{-2}	2.46313×10^{-1}
1.63541×10^{-1}	5.83575×10^{-1}
5.02989×10^{-1}	2.86373×10^{-1}
2.32350	4.36843×10^{-2}

$$J_p(\vec{K}_i,\alpha,\beta,\vec{K}_j)=\frac{3}{8}\frac{\pi^{3/2}}{\alpha^2\beta^2(\alpha+\beta)^{1/2}}\exp\left(-\frac{(\vec{K}_i-\vec{K}_j)^2}{4(\alpha+\beta)}\right)\times\left(\frac{(\vec{K}_i+\vec{K}_j)\cdot\vec{K}}{K^2}\left[\Phi(K\sqrt{\gamma})-1\right]+\vec{K}_i\cdot\vec{K}_j\,\Phi(K\sqrt{\gamma})+2\gamma\right)\ . \qquad (6)$$

With the help of the manageable analytic expressions (4) and (6) and a standard library program for the auxiliary Dawson function, we can easily evaluate the exchange bielectronic integrals. The other matrix elements appearing in the OPW method are simple[21]; the conduction energy bands of neon are obtained upon diagonalization of the OPW secular equation.

B. Energy bands of neon

Our computed Hartree-Fock conduction bands of neon are reported in Fig. 1. The irreducible representations of the little groups at symmetry points and symmetry lines are labeled following the notations of Ref. 22. Relevant crystal energies are given for convenience in Table II; energies

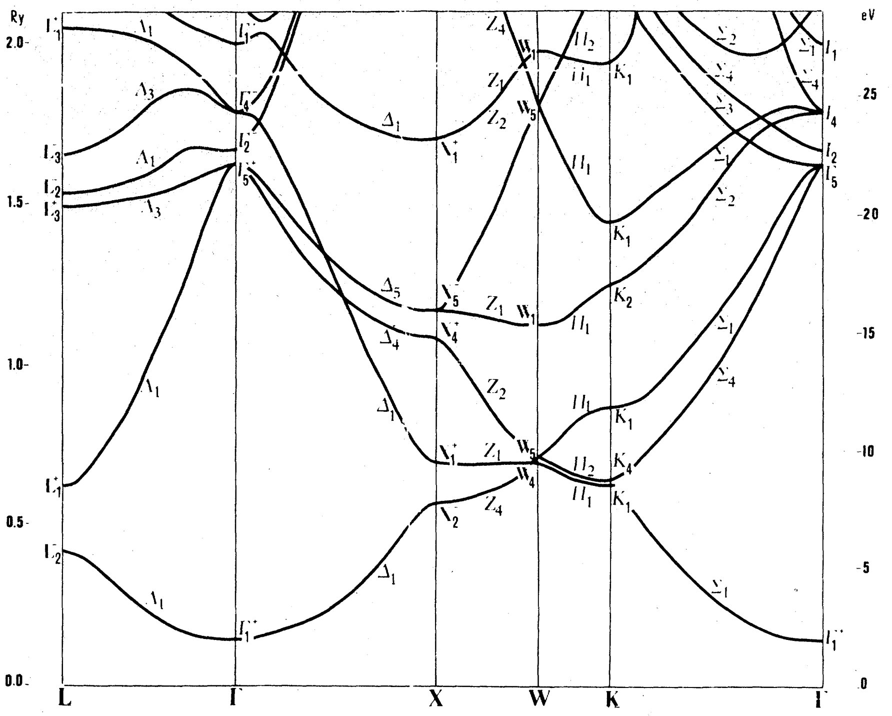

FIG. 1. Conduction energy bands of solid neon.

have been calculated at about 60 points, appropriately distributed in the Brillouin zone.

The results of Fig. 1 were obtained with a relatively small number (about 30) of plane waves orthogonalized to 1*s*, 2*s*, and 2*p* Bloch sums. To assess the reliability of these results, at a few selected symmetry points we set up the OPW method with orthogonalization only to the 1*s* Bloch sum with a much higher number (up to ≈150) of OPW's. We found that the 2*s* valence band rapidly approaches the energy of the 2*s* atomic state, but the convergence of the 2*p* band was very poor. This fact is similar to that observed by Lipari and Fowler[8] in the uppermost shell of argon. We explain this fact noting that the Fourier transform of a 2*s* function is less extended in $\vec{k}$ space than the Fourier transform of a 2*p* function (with the same screening parameter). Because of this convergence difficulty for the 2*p* band we decided to set up the OPW method with plane waves orthogonalized to 1*s* and 2*p* functions. With a high (but still acceptable) number of OPW's (about one hundred) we could both reproduce the 2*s* core band and test the reliability of the conduction bands reported in the work.

The general trend of the conduction bands of Fig. 1 can be easily understood by considering the empty lattice analysis for fcc structure and

TABLE II. Energies (in Rydberg) of relevant crystal states in solid neon at the points $\Gamma(\vec{k}=0)$, $X[\vec{k}=(2\pi/a)(1,0,0)]$, $L[\vec{k}=(2\pi/a)(\frac{1}{2},\frac{1}{2},\frac{1}{2})]$, and $K[\vec{k}=(2\pi/a)(\frac{3}{4},\frac{3}{4},0)]$ of the Brillouin zone.

Core and valence states / Conduction states	$E_{1s}=-62.99$	$E_{2s}=-3.568$	$E_{2p}=-1.585$
Γ_1^+ 0.146	X_2^- 0.565	L_2^- 0.418	K_1 0.627
Γ_5^+ 1.623	X_1^+ 0.692	L_1^+ 0.626	K_4 0.636
Γ_2^- 1.660	X_4^+ 1.083	L_3^+ 1.493	K_1 0.863
Γ_4^- 1.782	X_5^- 1.167	L_2^- 1.531	K_2 1.233
Γ_1^+ 1.989	X_1^+ 1.694	L_3^- 1.663	K_1 1.431
Γ_3^+ 2.154	X_3^+ 2.671	L_1^+ 2.054	K_1 1.931

observing that the empty lattice states with s-like and p-like symmetry feel the orthogonalization repulsive effects. Furthermore, since the screening parameters ξ_{2s} and ξ_{2p} are very close (actually they are taken as equal in Ref. 15), the effect of orthogonalization is expected to be more important for s like states than for p like states. This is essentially due to the l dependence of the orthogonalization coefficients.[21]

For instance, in the empty lattice analysis at point Γ, we have the level sequence $\mathbf{\Gamma}_1^+ \ll \mathbf{\Gamma}_1^+$, Γ_4^-, $\mathbf{\Gamma}_5^+$, Γ_2^-. The degeneracy of the empty lattice states $\mathbf{\Gamma}_1^+$, Γ_4^-, $\mathbf{\Gamma}_5^+$, $\mathbf{\Gamma}_2^-$ is removed, raising the energy of the s like state Γ_1^+ and p like state Γ_4^- with respect to $\mathbf{\Gamma}_5^+$ and Γ_2^-, and giving the expected sequence

$$\mathbf{\Gamma}_1^+ \ll \mathbf{\Gamma}_5^+, \ \Gamma_2^- < \Gamma_4^- < \Gamma_1^+ ,$$

which is in agreement with the detailed calculations. With similar arguments the expected sequence at X is

$$X_2^- < X_1^+ \ll X_4^+ < X_5^- < X_1^+ ,$$

while the expected sequence at L is

$$L_2^- < L_1^+ \ll L_3^+ < L_2^-, L_3^- < L_1^+ ,$$

again in agreement with the detailed calculations. Incidentally, we note that in argon and the other rare-gas solids, the difference in the screening parameters for s and p functions of the uppermost shell, the fact that orthogonalization effect to more extended functions are stronger, and the presence (in Kr and Xe) of d-core functions lead for conduction states to a sequence different from that peculiar to neon. Actually, in some symmetry points, neither the empty lattice sequence is maintained.

It is interesting to compare the results of the present calculation with those given in the literature (see Table III). From Table III, one can see that there is an overall agreement between different authors on the almost free-electron-like character of the conduction bands, but remarkable quantitative differences exist. Confining our attention to the two lowest conduction bands, we see, for instance, that all authors quoted in Table III agree that $L_2^- < L_1^+$, the difference being $E(L_1^+) - E(L_2^-) = 2.83$, 0.83, 0.62, 1.89, and 1.14 eV. For the difference $E(X_1^+) - E(X_2^-)$ we have instead 1.73, −0.99, −1.24, 5.1, and 3.16 eV for the authors cited in Table III.

If we take as an estimation of the width of the lower conduction band the energy difference between the lowest conduction state at X and the lowest conduction state at Γ, we have the following data (see Table III): 5.70 eV (present paper), 6.52 eV (Ref. 4), 6.71 eV (Ref. 5), 8.19 eV (Ref. 6), and 7.57 eV (Ref. 7). As a consequence, the effective conduction-band mass m_c^* at Γ is higher in the present paper. We have in fact $m_c^* = 1.27 m_e$ in the present calculation, against the values $m_c^* = 0.83 m_e$ of Rössler,[3] $m_c^* = 0.802 m_e$ of Kunz and Mickish,[6] and $m_c^* = 0.79 m_e$ of Natalizi and Resta.[5]

The currently available experimental data are in favor of the effective mass calculated in this paper, as can be seen from the following considerations. There is evidence that the interpretation of the higher members of the excitonic spectrum in neon require a reduced effective mass $\mu \simeq 0.8 m_e$. In our calculations we do not compute the width of the valence band (whose experimental value[23] is $\Delta_v = 1.3$ eV) because it is small with respect to the energy gap ($\simeq$ 21 eV).

TABLE III. HF conduction-band energies (in eV) of neon at some symmetry points by different authors.

	Present work	Dagens and Perrot (Ref. 4)	Natalizi and Resta (Ref. 5)	Kunz and Mickish (Ref. 6)	Euwema *et al.* (Ref. 7)
Γ_1^+	1.99	2.67	2.51	2.21	2.85
Γ_5^+	22.08	20.81	21.16		29.25
X_2^-	7.69	10.18	10.46	10.4	10.42
X_1^+	9.42	9.19	9.22	15.5	13.58
X_4^+	14.74	13.89	14.00		
X_5^-	15.88	17.84	18.38	19.8	18.28
L_2^-	5.69	7.92	8.15	8.10	8.38
L_1^+	8.52	8.75	8.77	9.99	9.52
L_3^+	20.31	19.21	19.53		

If, as in Ref. 14 we parametrize the dispersion of the valence band in the form

$$E_v(\vec{k}) = \frac{\Delta_v}{16}\left(12 - \sum_{\vec{\tau}_l}^{12} e^{i\vec{k}\cdot\vec{\tau}_l}\right) ,$$

at $\vec{k}=0$ we obtain for the average effective mass $m_v^* = 2.36 m_e$. The reduced effective mass between $m_c^* = 1.27 m_e$ and $m_v^* = 2.36 m_e$ gives $\mu = 0.82 m_e$, in agreement with the value deduced from the experimental binding energies of higher members of the excitonic series.

Before concluding this section we wish briefly to comment on the correlation effects on the Hartree-Fock band structure. Following the approximations and the notations of Ref. 14, we can estimate the correlation effects in rare-gas solids through the semiclassical relation

$$V_p(0) = (e^2/R_{\text{ML}})(1 - 1/\varepsilon_s) \simeq 1.3 \text{ eV},$$

where, for neon, the Mott-Littleton radius $R_{\text{ML}} = 4.18$ a.u. and $\varepsilon_s = 1.24$. Thus our HF energy gap (23.5 eV) corrected for the polarization effects gives a correlated energy gap (22.2 eV) in reasonable agreement with the experimental one (21.5 eV).

III. VALENCE AND CORE EXCITONS

In the last two years, powerful (and still numerically simple) approaches have been developed for studying excitons in closed-shell crystals and in particular in rare gases (see, for instance, Refs. 11, 13, and 14 and quoted references). All the mentioned papers exploit, though in a somewhat different theoretical framework, the accurately known atomic excitation energies to simplify the difficult-to-be-solved first-principle equations for excitons in crystals.

Following the procedure and the notations of Ref. 14, valence exciton binding energies and envelope functions are determined by the equation

$$[E_c(-i\nabla) + E_v(-i\nabla) + V_h(r) + V_c(r) + V_p(r)]\Phi(\vec{r}) = E\Phi(\vec{r}) , \quad (7)$$

where $E_c(\vec{k})$ is the conduction-band energy (measured from $\vec{k}=0$), $E_v(\vec{k})$ is the valence-band energy (measured form $\vec{k}=0$ and positive sign), $V_h(r)$ is the hole Coulomb potential, $V_c(r)$ is the "central cell" correction potential determined by exploiting experimental atomic energies, and $V_p(r)$ is the polarization potential. For core excitons, a similar equation applies except that $E_v(\vec{k})$ has to be omitted.

The parametrization of the energy bands and the expression for $V_h(r)$, $V_c(r)$, and $V_p(r)$ have been obtained following step by step the procedures of Ref. 14. However, a more accurate account of the "band kinetic operator" $E_c(-i\nabla) + E_v(-i\nabla)$ is provided here with the following variational method.

Consider first the Schrödinger equation

$$[-\hbar^2\nabla^2/2m^* + V_h(r) + V_c(r) + V_p(r)]F(\vec{r}) = E_0 F(\vec{r}) , \quad (8)$$

which is obtained from (7) by replacing the complicated operator $E_c(-i\nabla) + E_v(-i\nabla)$ by the standard kinetic operator $-\hbar^2\nabla^2/2m^*$ with a given value of the effective-mass parameter m^*. The above equation is solved numerically with standard programs[16] for various values of m^*. Let us indicate with $F_{1s}(m^*, \vec{r})$ and $E_{1s}^0(m^*)$ the wave functions and eigenvalues of Eq. (8) corresponding, for instance, to the $1s$ state. The set of functions $F_{1s}(m^*, \vec{r})$ are used variationally to minimize the energy

$$\begin{aligned} E_{1s}(m^*) &= \langle F_{1s}(m^*, \vec{r}) \,|\, [E_c(-i\nabla) + E_V(-i\nabla) + V_h(r) + V_c(r) + V_p(r)] \,|\, F_{1s}(m^*, \vec{r}) \rangle \\ &= E_{1s}^0(m^*) + \left\langle F_{1s}(m^*, \vec{r}) \middle| \left[E_c(-i\nabla) + E_v(-i\nabla) - \left(-\frac{\hbar^2\nabla^2}{2m^*}\right)\right] \middle| F_{1s}(m^*, \vec{r}) \right\rangle \\ &= E_{1s}^0(m^*) + \int |F_{1s}(m^*, \vec{k})|^2 \left(E_c(\vec{k}) + E_v(\vec{k}) - \frac{\hbar^2 k^2}{2m^*}\right) d\vec{k} , \end{aligned} \quad (9)$$

where $F_{1s}(m^*, \vec{k})$ is the Fourier transform of $F_{1s}(m^*, \vec{r})$. In order to evaluate with accuracy the integral appearing in Eq. (9), we have found it convenient to expand the function $F_{1s}(m^*, r)$, which is known numerically, into basis functions

$$L_n(\alpha r)e^{-\alpha r/2} \quad \text{with } \tfrac{1}{2}\alpha = [2m^* E_{1s}^0(m^*)]^{1/2}$$

and $L_n(x)$ Laguerre polynomial of order n. In our case it was more than sufficient to take n up to 5. Since the Fourier transform of a polynomial times an exponential function is analytic, the integral appearing in Eq. (9) can be performed with high accuracy and little labor. As an example, we report in Fig. 2 the behavior of $E_{1s}^0(m^*)$

TABLE IV. Experimental and theoretical valence and core exciton energies in gaseous and solid neon.

Exciton series	Envelope function notations	Expt. transition energies in the gas (Refs. 17 and 18)	Expt. binding energies in the gas	Calc. binding energies in the gas	Expt. transition energies in the solid (Refs. 24 and 25)	Expt. binding energies in the solid	Calc. binding energies in the solid
valence	1s	16.666	−4.893	−4.892	17.59	−3.95	−3.72
excitons	2s	19.683	−1.876	−1.893	20.25	−1.29	−1.20
$2p_{3/2}\to(n+2)s$	3s	20.565	−0.994	−1.002	20.92	−0.62	−0.59
	4s	20.944	−0.615	−0.619	21.18	−0.36	−0.36
	5s	21.141	−0.418	−0.421	21.29	−0.25	−0.25
		edge 21.559			estimated edge 21.54		
core 2s	2p	45.546	−2.922	−2.922	46.92	−2.13	−2.35
excitons	3p	47.121	−1.347	−1.348	48.00	−1.05	−1.05
	4p	47.692	−0.776	−0.777			−0.56
	5p	47.965	−0.503	−0.503			−0.43
		edge 48.468			estimated edge 49.05		

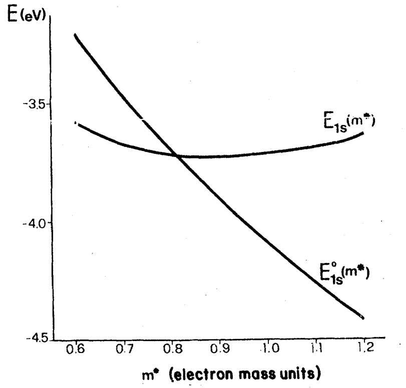

FIG. 2. Computation of the binding energy of 1s valence exciton in solid neon. Energies are in eV and m^* in electron mass units. $E^0_{1s}(m^*)$ is the 1s eigenvalue of Eq. (8) and $E_{1s}(m^*)$ is provided by Eq. (9).

for the valence 1s exciton of neon. It can be seen that while $E^0_{1s}(m^*)$ is very sensitive to the chosen value of m^*, $E_{1s}(m^*)$ is instead insensitive to it.

In Table IV we report, for comparison, experimental and theoretical valence and core excitation energies in gaseous and solid neon. The experimental excitation energies for the gas are taken from Refs. 17 and 18. The 2s core excitonic spectrum of solid neon is taken from Ref. 24. The valence excitonic spectrum of solid neon has been investigated by several authors (see, for instance, Refs. 2, 25 and 26 and references quoted therein); in particular, a lot of interest has been devoted to the $n=1$ exciton (see, for instance, Refs. 10 and 27 and references quoted therein). From Table IV we see that the agreement between experimental and calculated values is good. However, some discrepancies are found in experiments in the case of the $n=1$ excitonic transition. A thorough and detailed understanding of the 1s exciton probably needs further work on the experimental and theoretical side.

IV. CONCLUSIONS

In this paper we have adopted a modified orthogonalized plane-wave method to calculate the energy bands of solid neon. An accurate and numerically simple account of the electronic exchange potential is obtained using the Gaussian representation of atomiclike orbitals. The band structure is found to be consistent with the experimental valence and core exciton spectra. The method and procedures of this paper should find wide application and allow a better comprehension of the electronic structure and excitonic effects in a number of large-gap insulators.

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