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LETTER TO THE EDITOR

A method of calculating k -dependent positron states based on the finite-difference approximation

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Abstract. A method for solving the k -dependent positron Schrödinger equation has been developed, extending the numerical technique developed by Puska and Nieminen. It is possible to apply the present method to calculations of the positron band mass m^* . Results for alkali metals and $\text{YBa}_2\text{Cu}_3\text{O}_7$ are presented as examples.

The numerical solution of the Schrödinger equation was originally developed by Kimball and Shortley [1] and applied to positron problems by Puska and Nieminen [2]. The differential equation

$$-\frac{1}{2}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{1}$$

is replaced by a set of linear algebraic equations on three-dimensional mesh points:

$$-\frac{1}{2}\left(\frac{\psi_{i+1,j,k} - 2\psi_{i,j,k} + \psi_{i-1,j,k}}{h_x^2} + \frac{\psi_{i,j+1,k} - 2\psi_{i,j,k} + \psi_{i,j-1,k}}{h_y^2} + \frac{\psi_{i,j,k+1} - 2\psi_{i,j,k} + \psi_{i,j,k-1}}{h_z^2}\right) + V_{i,j,k}\psi_{i,j,k} = E\psi_{i,j,k} \tag{2}$$

The atomic unit is used throughout. Each mesh point is represented by three integers. $\psi_{i,j,k}$ and $V_{i,j,k}$ are values of the positron wavefunction and potential at the point (i, j, k) . h_x , h_y and h_z are mesh spacings for the x , y and z directions, respectively. In this case, the energy eigenvalue $E = \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle$ (H : Hamiltonian) can be obtained from the following equation:

$$E = \sum_{i,j,k} \left[f_{i,j,k} \left\{ -\frac{1}{2}\psi_{i,j,k} \left(\frac{\psi_{i+1,j,k} + \psi_{i-1,j,k}}{h_x^2} + \frac{\psi_{i,j+1,k} + \psi_{i,j-1,k}}{h_y^2} + \frac{\psi_{i,j,k+1} + \psi_{i,j,k-1}}{h_z^2} \right) + \left(\frac{1}{h_x^2} + \frac{1}{h_y^2} + \frac{1}{h_z^2} + V_{i,j,k} \right) \psi_{i,j,k}^2 \right\} \right] / \sum_{i,j,k} f_{i,j,k} \psi_{i,j,k}^2 \tag{3}$$

where $f_{i,j,k}$ is a weight factor. For an orthorhombic system, $f_{i,j,k} = 1$ inside the unit cell, $1/2$ on the boundary planes, $1/4$ on the edges and $1/8$ at the corners. Setting $\partial E / \partial \psi_{i,j,k} = 0$, a set of equations

$$\psi_{i,j,k} = \frac{(\psi_{i+1,j,k} + \psi_{i-1,j,k})/h_x^2 + (\psi_{i,j+1,k} + \psi_{i,j-1,k})/h_y^2 + (\psi_{i,j,k+1} + \psi_{i,j,k-1})/h_z^2}{2(1/h_x^2 + 1/h_y^2 + 1/h_z^2 + V_{i,j,k} - E)} \tag{4}$$

are obtained. The wavefunction is optimized by iterations of calculations of new values of E and $\psi_{i,j,k}$.

The above technique can be applied to both bulk and trapped states of positrons with appropriate boundary conditions. For the bulk state with $k = 0$, the condition is that the first normal derivative of the wavefunction on the surface of the Wigner-Seitz polyhedron (or the unit cell) vanishes. For the trapped state, the wavefunction itself is required to vanish on the boundary surface far enough from the trap site. It is possible to calculate other k states by using proper boundary conditions which depend on the wave vector k and the symmetry, as Puska *et al* did for hydrogen and helium atoms in metals and on surfaces [3-5].

In the present work, a new technique for calculating k -dependent positron states is demonstrated. Instead of dealing with rather complicated boundary conditions, the wave vector k is incorporated explicitly in the Schrödinger equation and the expressions for energy and wavefunction values in the finite-difference approximation. The periodic boundary condition is applied in this case. As an application, positron effective masses m^* are calculated for a few materials.

To calculate positron states for general k , a complex Bloch function

$$\varphi_k(\mathbf{r}) = \varphi(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \quad (5)$$

has to be introduced. The k -dependent Schrödinger equation is reduced to

$$-\frac{1}{2}\nabla^2\varphi(\mathbf{r}) - i\mathbf{k} \cdot \nabla\varphi(\mathbf{r}) + \left(\frac{|\mathbf{k}|^2}{2} + V(\mathbf{r})\right)\varphi(\mathbf{r}) = E\varphi(\mathbf{r}). \quad (6)$$

Applying the finite-difference approximation, E is represented by

$$E = \sum_{i,j,k} \left[-f_{i,j,k} \left\{ -\frac{\varphi_{i,j,k}^R \varphi_{i+1,j,k}^R + \varphi_{i,j,k}^I \varphi_{i+1,j,k}^I}{h_x^2} - \frac{\varphi_{i,j,k}^R \varphi_{i,j+1,k}^R + \varphi_{i,j,k}^I \varphi_{i,j+1,k}^I}{h_y^2} \right. \right. \\ \left. - \frac{\varphi_{i,j,k}^R \varphi_{i,j,k+1}^R + \varphi_{i,j,k}^I \varphi_{i,j,k+1}^I}{h_z^2} + \frac{k_x(\varphi_{i,j,k}^R \varphi_{i+1,j,k}^I - \varphi_{i,j,k}^I \varphi_{i+1,j,k}^R)}{h_x} \right. \\ \left. + \frac{k_y(\varphi_{i,j,k}^R \varphi_{i,j+1,k}^I - \varphi_{i,j,k}^I \varphi_{i,j+1,k}^R)}{h_y} + \frac{k_z(\varphi_{i,j,k}^R \varphi_{i,j,k+1}^I - \varphi_{i,j,k}^I \varphi_{i,j,k+1}^R)}{h_z} \right. \\ \left. + \left(\frac{1}{h_x^2} + \frac{1}{h_y^2} + \frac{1}{h_z^2} + \frac{|\mathbf{k}|^2}{2} + V_{i,j,k} \right) |\varphi_{i,j,k}|^2 \right] / \sum_{i,j,k} f_{i,j,k} |\varphi_{i,j,k}|^2 \quad (7)$$

$$\varphi_{i,j,k} = \varphi_{i,j,k}^R + i\varphi_{i,j,k}^I \quad (\varphi_{i,j,k}^R, \varphi_{i,j,k}^I : \text{real}) \quad (8)$$

$$\mathbf{k} = (k_x, k_y, k_z). \quad (9)$$

Setting $\partial E / \partial \varphi_{i,j,k}^R = 0$ and $\partial E / \partial \varphi_{i,j,k}^I = 0$, the following two equations are obtained:

$$\varphi_{i,j,k}^R = \left[\frac{\varphi_{i+1,j,k}^R + \varphi_{i-1,j,k}^R}{h_x^2} + \frac{\varphi_{i,j+1,k}^R + \varphi_{i,j-1,k}^R}{h_y^2} + \frac{\varphi_{i,j,k+1}^R + \varphi_{i,j,k-1}^R}{h_z^2} \right. \\ \left. - \frac{k_x(\varphi_{i+1,j,k}^I - \varphi_{i-1,j,k}^I)}{h_x} - \frac{k_y(\varphi_{i,j+1,k}^I - \varphi_{i,j-1,k}^I)}{h_y} - \frac{k_z(\varphi_{i,j,k+1}^I - \varphi_{i,j,k-1}^I)}{h_z} \right] \\ \times \left(\frac{2}{h_x^2} + \frac{2}{h_y^2} + \frac{2}{h_z^2} + |\mathbf{k}|^2 + 2V_{i,j,k} - 2E \right)^{-1} \quad (10)$$

$$\varphi_{i,j,k}^I = \left[\frac{\varphi_{i+1,j,k}^I + \varphi_{i-1,j,k}^I}{h_x^2} + \frac{\varphi_{i,j+1,k}^I + \varphi_{i,j-1,k}^I}{h_y^2} + \frac{\varphi_{i,j,k+1}^I + \varphi_{i,j,k-1}^I}{h_z^2} \right. \\ \left. + \frac{k_x(\varphi_{i+1,j,k}^R - \varphi_{i-1,j,k}^R)}{h_x} + \frac{k_y(\varphi_{i,j+1,k}^R - \varphi_{i,j-1,k}^R)}{h_y} + \frac{k_z(\varphi_{i,j,k+1}^R - \varphi_{i,j,k-1}^R)}{h_z} \right] \\ \times \left(\frac{2}{h_x^2} + \frac{2}{h_y^2} + \frac{2}{h_z^2} + |\mathbf{k}|^2 + 2V_{i,j,k} - 2E \right)^{-1} \quad (11)$$

The equations (7) and (10) correspond to the equations (3) and (4), respectively, in the case where $k = 0$ and $\varphi_{i,j,k}$ is real.

According to the above formulation, positron energy eigenvalues as functions of \mathbf{k} are calculated for alkali metals and $\text{YBa}_2\text{Cu}_3\text{O}_7$. The positron potential $V(\mathbf{r})$ is constructed using a method based on the superposed atom model [2] as

$$V(\mathbf{r}) = V_C(\mathbf{r}) + V_{\text{corr}}(n_-(\mathbf{r})) \quad (12)$$

where V_C is the Coulombic part from nuclei and electrons while V_{corr} is the correlation potential due to positron-electron (e^+e^-) correlation effects. The practical form of V_{corr} as a function of $n_-(\mathbf{r})$ was given by Boroński and Nieminen [6]. $n_-(\mathbf{r})$ and $V_C(\mathbf{r})$ were obtained by the superposition of neutral-atom electron densities and potentials [7]. The values $E(\mathbf{k})$ have been calculated in the vicinity of the Γ point along the [001] axis for alkali metals ($0 \leq k_x \leq 0.005 \times 2\pi/a$) and along the [100], [010] and [001] axes for $\text{YBa}_2\text{Cu}_3\text{O}_7$ ($0 \leq k_x \leq 0.005 \times 2\pi/a$, $0 \leq k_y \leq 0.005 \times 2\pi/b$, $0 \leq k_z \leq 0.005 \times 2\pi/c$). The mesh spacings are $a/20$ for alkali metals and $a/20$, $b/20$ and $c/60$ for $\text{YBa}_2\text{Cu}_3\text{O}_7$. As for K, additional calculations have been done with mesh spacings of $a/10$ and $a/40$ to check the convergence, and along the [011] and [111] axes to confirm the symmetry. The positron band mass m^* is obtained by fitting the resultant $E(\mathbf{k})$ curve to a parabola. The values obtained are listed in table 1 together with the calculation conditions.

Table 1. Positron band masses calculated on the basis of the finite-difference approximation.

Material	Band mass m^*	Axis \mathbf{k}	Mesh spacing
Li	1.0210	[001]	$a/20$
Na	1.0288	[001]	$a/20$
K	1.0419	[001]	$a/20$
	1.0389	[001]	$a/10$
	1.0427	[001]	$a/40$
	1.0419	[011]	$a/20$
	1.0419	[111]	$a/20$
Rb	1.0477	[001]	$a/20$
Cs	1.0565	[001]	$a/20$
$\text{YBa}_2\text{Cu}_3\text{O}_7$	1.1631	[100]	$a/20, b/20, c/60$
	1.0658	[010]	
	2.2441	[001]	
$\text{YBa}_2\text{Cu}_3\text{O}_7$	1.3135	[100]	$a/20, b/20, c/60$
No e^+e^- correlation	1.0716	[010]	
	5.9151	[001]	

Comparing m^* values for K along the [001] axis calculated for various mesh spacings, it can be concluded that the mesh spacing $a/20$ is fine enough because the difference from

the value for $a/40$ is at most 0.1%. The masses along [001], [011] and [111] are the same. This does not conflict with the expected s-like character of the cubic symmetry.

The values obtained for the positron band mass m^* in various alkali metals are almost unity, although they increase slightly with the lattice constant increasing in going from Li to Cs. This is in good agreement with previous reports [8–10]. These band masses are significantly smaller than the effective masses obtained experimentally in which other contributions such as phonon effects are included [8, 11–14].

$\text{YBa}_2\text{Cu}_3\text{O}_7$ is a typical anisotropic compound and thought to be a good example for showing an anisotropic band mass. Von Stetten *et al* calculated the positron band mass on $\text{YBa}_2\text{Cu}_3\text{O}_7$ by the self-consistent LAPW method and obtained the values of 1.17 along [100], 1.05 along [010] and 6.6 along [001] [15]. Their value along the [001] axis is much larger than that of the present work. In their calculation, the e^+e^- correlation was not included. In order to compare with their result more appropriately, the band mass is calculated with no e^+e^- correlation term included in the potential. The resultant values are also listed in table 1. The agreement with the results of von Stetten *et al* [15] is rather good in this case. Whether or not the correlation is included, the calculated positron distribution shows its density maximum between one-dimensional Cu–O chains. The amplitude of the positron density decreases along the [001] axis more rapidly in the case where the correlation is not included, however. The present results are consistent with the previous calculations made by von Stetten *et al* and Singh *et al* [16]. The remarkable change of the band mass along the [001] axis reflects the above-mentioned difference in the positron density.

In summary, a method for obtaining k -dependent positron states is presented. As an application, positron band masses m^* have been calculated for alkali metals and $\text{YBa}_2\text{Cu}_3\text{O}_7$.

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References

- [1] Kimball G E and Shortley G H 1934 *Phys. Rev.* **45** 815
- [2] Puska M J and Nieminen R M 1983 *J. Phys. F: Met. Phys.* **13** 333
- [3] Puska M J and Nieminen R M 1984 *Phys. Rev. B* **29** 5382
- [4] Puska M J and Nieminen R M 1983 *Phys. Rev. Lett.* **51** 1081
- [5] Puska M J and Nieminen R M 1985 *Surf. Sci.* **157** 413
- [6] Boroński E and Nieminen R M 1986 *Phys. Rev. B* **34** 3820
- [7] Herman F and Skillman S 1963 *Atomic Structure Calculations* (Englewood Cliffs, NJ: Prentice-Hall)
- [8] Stewart A T, Shand J B and Kim S M 1966 *Proc. Phys. Soc.* **88** 1001
- [9] Majumdar C K 1966 *Phys. Rev.* **149** 406
- [10] Stott M J and Kubica P 1975 *Phys. Rev. B* **11** 1
- [11] For a review, see
Berko S 1983 *Positron Solid-State Physics* ed W Brandt and A Dupasquier (Amsterdam: North-Holland) p 64
- [12] Kim S M and Stewart A T 1975 *Phys. Rev. B* **11** 2490
- [13] Kubica P and Stewart A T 1975 *Phys. Rev. Lett.* **34** 852
- [14] Hyodo T, McMullen T and Stewart A T 1986 *Phys. Rev. B* **33** 3050
- [15] von Stetten E C, Berko S, Li X S, Lee R R, Brynstad J, Singh D, Krakauer H, Pickett W E and Cohen R E 1988 *Phys. Rev. Lett.* **60** 2198
- [16] Singh D, Pickett W E, Cohen R E, Krakauer H and Berko S 1989 *Phys. Rev. B* **39** 9667