Scientific Research Publishing

Journal of Applied Mathematics and Physics, 2022, 10, 2407-2414
https://www.scirp.org/journal/jamp
ISSN Online: 2327-4379
ISSN Print: 2327-4352

Towards a Novel Super Current

Hubert Klar

Retired from University Freiburg, Freiburg, Germany
Email: hubklar@aol.com

How to cite this paper: Klar, H. (2022) Towards a Novel Super Current. *Journal of Applied Mathematics and Physics*, **10**, 2407-2414.
https://doi.org/10.4236/jamp.2022.107163

Received: June 23, 2022
Accepted: July 26, 2022
Published: July 29, 2022

Abstract

For nonrelativistic two-electron atoms, we employ a phase-amplitude method to derive an energy-dependent three-body force which controls the dynamics of the atom near the threshold for double escape. Its potential energy has been taken into account to derive beyond a static adiabatic basis a novel partial differential equation that replaces an adiabatic basis. That equation whose solutions span a Banach space has been solved exactly in the energy window near threshold. In that energy range, we find the formation of unstable electron pairs, comparable to Cooper pairs. In contrast to Cooper pairs, our pairs are bound by dominant correlation rather than by the coupling to a phonon field. These ingredients are suspected to allow for a super current independent of the temperature.

Keywords

Correlation, Wannier Theory, Evolution, Superconductivity

1. Introduction

Superconductivity, experimentally known since a long time, see [1], got only much later a theoretical explanation by Bardeen *et al.* [2] usually referred to as BCS theory. The key ingredient of this theory is the formation of electron pairs. The attractive force between two electrons emerges from the coupling of the electrons motion to the lattice vibration, usually referred to as electron-phonon interaction. Therefore superconductivity works only at extremely low temperatures (few Kelvin). Some materials show high temperature superconductivity, shortly HTS. Actually, however, these "high temperatures" are still much below room temperature. Presently we are still away from superconductivity at room temperature although several designs have been proposed in the past to open the way to superconductivity at room temperature [3] [4] [5].

2. Ingredients of the Theory

It is the aim of this comment to present an electron pair formation mechanism

independent of the temperature and therefore different from Cooper pairs. We will see shortly that dominant electron correlation in a restricted energy window does allow for an unstable attraction between electrons. Before we enter into details of the new achievement we list necessary ingredients for the development of the theory.

To this end we go back to Wannier's threshold ionization theory [6]. He considers two electrons in the field of a point nucleus with charge *Z*. The electrostatic potential energy is then for not too heavy nuclei given by

$$V = -Z\left(\frac{1}{r_1}+\frac{1}{r_2}\right)+\frac{1}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\Theta}} \tag{1}$$

where the $r_i\,(i=1,2)$ are the electron-nucleus distances and Θ is the solid angle bewen the electrons directions. We remark that this angle is restricted to $0\le\Theta\le\pi$, because larger angles $\Theta'>\pi$ may be replaced by $2\pi-\Theta'<\pi$. In order to study radial correlation Wannier [6] parameterizes the radial distances by introducing a pseudo angle α given by

$$\alpha = \tan^{-1}\frac{r_1}{r_2} \tag{2}$$

with $0\le\alpha\le\pi/2$
and the so called hyperradius

$$R=\sqrt{r_1^2+r_2^2} \tag{3}$$

The potential (1) reads in these coordinate

$$V=\frac{C(\alpha,\theta)}{R} \tag{4}$$

the charge function $C(\alpha,\Theta)$ given by

$$C(\alpha,\Theta)=-2Z\sqrt{2}\frac{\cos(\alpha-\pi/4)}{\sin 2\alpha}+\frac{1}{\sqrt{1-\sin 2\alpha\cos\Theta}} \tag{5}$$

Wannier claims that the charge function has a saddle point located at $\alpha=\pi/4$ and $\Theta=\pi$. He identifies the saddle point from the Taylor expansion centered at $(\pi/4,\Theta=\pi)$

$$C(\alpha,\theta)=-C_0+C_1(\theta-\pi)^2-C_2\left(\alpha-\frac{\pi}{4}\right)^2$$

Since C_1 is small and does not contribute to the threshold ionization law, we fix below $\theta=\pi$, or alternatively we put a smooth θ dependence into C_2. *i.e.* we use below the expansion

$$C(\alpha,\theta)=-C_0-C_2(\alpha-\pi/4)^2 \tag{6}$$

Thus we arrive at the coefficients are given by

$$C_0=2\sqrt{2}Z-\frac{1}{\sqrt{1-\cos\theta}} \tag{7}$$

$$C_2 = 3 + \frac{\cos\theta}{(1-\cos\theta)^{3/2}} \tag{8}$$

The graph of the Expansion (6) describes a local maximum along the coordinate α. The constant C_2 represents then the curvature in its maximum whereas the constant C_0 is the charge of the electron pair in the maximum.

Geometrically the potential energy surface $V = C/R$, see (4), represents a potential ridge along an evolution coordinate R, the maximum of the ridge is located at $\alpha = \pi/4$. The width of the ridge depends on the angel θ. For not too small angles θ both constants are positive. This implies that the whole potential surface puts the electron pair into an unstable equilibrium.

We go now beyond the classical Wannier work to treat the problem quantum mechanically [7]. In terms of the above coordinates the stationary wave equation linearized in the coordinate α at the equilibrium point $\alpha = \pi/4$ reads

$$\left\{-\frac{1}{2}\frac{\partial^2}{\partial R^2} - \frac{1}{2R^2}\frac{\partial^2}{\partial \beta^2} + \frac{15/4}{2R^2} - \frac{C_0}{R} - \frac{C_2}{R}\beta^2 - E\right\}\left\{R^{-5/2}\Psi\right\} = 0 \tag{9}$$

with

$$\beta = \alpha - \frac{\pi}{4} \tag{10}$$

Equation (9) is not separable. We show below that near threshold exists a solution in form of a semiclassical phase-amplitude solution. Due to the smoothness of Coulomb interactions we expect solutions in Eikonal form

$$\Psi = R^{5/2}A(R)\exp\{iS\} \tag{11}$$

S being the classical action. We conclude from the radial kinetic energy

$$-\frac{1}{2}\frac{\partial^2}{\partial R^2}A = -\frac{1}{2}A'' - A'\frac{\partial}{\partial R} - \frac{1}{2}A\frac{\partial^2}{\partial R^2} \tag{12}$$

Since near threshold we expect a smooth amplitude A, we reject its second derivative A''. To the Wannier phenomenon [7] contribute only long-range Coulomb interactions like the static Coulomb potential (4). We stress that (12) delivers another $1/R$ term hidden in the kinetic energy. That is the first derivative term A' in (12) which may be rewritten as follows

$$-A'\frac{\partial}{\partial R} = -\frac{A'}{A}A\frac{\partial}{\partial R} = -iK(R)A\frac{\partial}{\partial R} \tag{13}$$

In (13) we have employed the boundary condition for the logarithmic derivative on the top of the ridge, in detail

$$K(R) = \pm\sqrt{2\left(E + \frac{C_0}{R}\right)} \tag{14}$$

which becomes at threshold $E = 0$

$$K(R) = \pm\sqrt{\frac{2C_0}{R}} \tag{15}$$

Our improved channel wave Equation (9) reads therefore in the Coulomb zone

$$\left\{\mp i\sqrt{\frac{2C_0}{R}}\frac{\partial}{\partial R}-\frac{1}{2R^2}-\frac{\partial^2}{\partial\beta^2}-\frac{C_0}{R}-\frac{C_2}{R}\beta^2-E\right\}\Phi(\beta,R)=0 \tag{16}$$

where we have rejected powers R^{η} with $\eta<-1$.

The last steps deserve some comments. The traditional treatment of the two-electron problem starts from a Born-Oppenheimer basis [8] [9]. Non-adiabatic couplings must then be taken into account. That procedure is rather slow moving because an infinite number of collision channels must be taken into account what in fact is impossible because an infinite number of channels converges to the ionization threshold [10].

We present here an alternative way. We circumvent the adiabatic channel expansion, and derive directly from the kinetic energy operator a novel energy-dependent three-body interaction, see also [11]. Along these lines we have arrived at an entirely new partial differential Equation (16) which replaces the familiar adiabatic basis. We stress that this new wave Equation (16) is a parabolic partial differential equation although we started from an elliptic one. Our (16) is a transport equation comparable to the heat equation. The transported material is in our case a two-electron charge density, the transport itself occurs via wave diffraction.

The first term in (16), entirely foreign to standard atomic theory, constitutes a three-body-Coulomb-interaction which deforms the static Coulomb potential surface (4). We stress that a three-body-interaction manifests itself by the fact that it cannot be represented by a sum of three two-body interactions. That may be seen as follows. It is evident that the classical action for our Coulomb system is $\propto\sqrt{R}$ where R is the hyperradius. Therefore we get

$$\mp i\sqrt{\frac{2C_0}{R}}\frac{\partial}{\partial R}\Phi\propto\mp i^2\frac{1}{R}\sqrt{\frac{C_0}{2}}D(\alpha)\Phi=\pm\frac{\sqrt{C_0/2}}{R}D(\beta)\Phi \tag{17}$$

provided we write the exponential in (11) in the form

$$\Phi\propto\exp\left\{i\sqrt{R}D(\alpha)\right\} \tag{18}$$

Below we combine the two Coulomb potentials (4) plus (16) to one new modified Coulomb potential given by

$$\frac{C(\beta)\pm D(\beta)\sqrt{C_0/2}}{R} \tag{19}$$

We stress that the deformation term depends on the direction of a two-electron wave propagation, typical for a fictitious force. The presence of a fictitious force is here not unexpected since we describe the angular motion (β) in a moving frame along the evolution R.

We complete the non-adiabatic treatment with the calculation of the modified action portion $D(\beta)$. To this end, we use in our model a quadratic Ansatz given by

$$D(\beta) = \kappa + \mu\beta^2 \tag{20}$$

With (16)-(19) we find immediately

$$\kappa = \sqrt{2C_0} \tag{21}$$

and two solutions for μ given by

$$\mu^+ = \frac{1}{4}\left(\sqrt{\frac{C_0 + 16C_2}{2}} - \sqrt{\frac{C_0}{2}}\right) > 0 \tag{22}$$

$$\mu^- = -\frac{1}{4}\left(\sqrt{\frac{C_2 + 16C_2}{2}} + \sqrt{\frac{C}{2}}\right) < 0 \tag{23}$$

The indices +/− refer to contraction/expansion of the whole three-body complex; analogous to incoming/outgoing waves in the familiar two-body case. The contraction wave describes in our three-body system a pair of dominantly correlated electrons approaching the nucleus. It is obvious that the electrons attract each other during their correlated path to the nucleus. This resembles to Coopper pairs except that Cooper's electron-phonon interaction has been replaced in our treatment by the electron-nucleus interaction.

The evolution

$$\Phi(\alpha, R) = A\exp\left\{i\sqrt{R}\left\langle \lambda + \mu\beta^2 \right\rangle\right\} \tag{24}$$

constitutes a Fresnel distribution [11], and has an important property. It solves initial value-problems. The **Appendix** of this paper shows that an evolution like (24) converges at $R \to \infty$ up to a constant factor to a delta distribution $\propto \delta(\beta)$. It solves therefore the channel Equation (16). It constitutes therefore a kernel of (16) and delivers solutions of (9) in the form

$$\Phi\left(\beta, R; \mu^{\pm}\right) = \int_{-\pi/4}^{+\pi/4} \mathrm{d}\beta' \, \Phi_0^{\pm}\left(\beta', R; \mu^{\pm}\right) \exp\left\{i\sqrt{R}\left(\lambda + \mu^+\left(\beta - \beta'\right)\right)^2\right\} \tag{25}$$

provided $\Phi_0^{\pm}$ is an initial value state. The existence of two kinds of evolutions, distinguished by the parameters $\mu^{\pm}$, compares favorably with Wannier's classical results. He has reported two sorts of trajectories, a converging one and a diverging one. These correspond one to one to our two evolutions presented here.

3. Mechanism of Charge Transport

We have now all ingredients for a charge transport design through a multiatomic system; a transport which does not suffer from energy loss due to inelastic collisions. For simplicity we consider a linear chain of identical atoms with one valence electron, the nuclei separated by a lattice constant *a*. We label the atoms in the chain by #1, #2, and so on. W*e* investigate at first a charge transport from #1 to #2 in three steps.

Step 1: We hit for instance atom #1 by a slow electron. Its energy should be only little (typically < 3 eV) below the ionization threshold of the valence target electron.

As soon as the electron enters the 3-body-Coulomb zone the motion of the

target electron plus the scattering electron is controlled by the Fresnel distribution (25) with the parameter μ^+, see (22). With the initial boundary condition $\Phi(\beta' = \text{arbitrary for } R \to \infty)$ we get at finite values of R a channel function $\propto \int_{-\pi/4}^{+\pi/4} \mathrm{d}\beta' \Phi(\beta'; R) \exp\left(i\sqrt{R}\mu^+ (\beta - \beta')^2\right) \to \Phi(\beta \approx 0; R)$. *i.e.* during that step the complex performs a contraction in which the electrons attract each other: as it was schematically displayed on the basis of classical trajectories in [6]. The electrons, however, do not fall into the nucleus because of the static resulsive barrier given by

$$+\frac{15}{8R^2} \tag{26}$$

see (9) which constitutes a centrifugal potential universal for all doubly excited target atoms although there is no rotation at all.

Step 2:

The barrier has played the role of a mirror: It reflects the two-electron wave. The expanding complex is now controlled by the parameter μ^- which causes the decay of the pair due to the instability of that mode. One electron is trapped into the valence from where it came from whereas the other one escapes. So easy, however, is the situation in the case of one nucleus only, see step #3 below.

Step 3: To this end we remark that the way out meets a dynamical zero of the evolution. That unusual feature may be seen by looking to the conservation of energy on the top of the ridge, *i.e.* at $\alpha = \pi/4$. The total energy reads then

$$E = \frac{1}{2}\dot{R}^2 - \frac{C_0}{R} \tag{27}$$

Inspection of (27) shows that for negative values of the energy E the radial velocity has a zero located at a critical radius given by

$$R_c = \frac{C_0}{|E|} \tag{28}$$

see (7) with $C_0 > 0$, for not too small angles θ. That critical radius did not occur in Wannier's study at $E > 0$. If the escaping wave reaches the sphere with radius R_c it comes to rest. It experiences two possibilities: either the wave is reflected to its mother nucleus or it continues the way out as uncorrelated electron. If the critical radius R_c is larger than $a/2$. the two spheres overlap at least partially. The reflected electron may therefore arrive in the frame of atom #2. In a realistic experimental setup more electrons will have taken the same way. A return to atom #1 is then forbidden by the Pauli principle if the follow electron has already occupied the Wannier orbital. Note that all atoms have the same critical radius at the same energy. The initially outgoing electron controlled by the parameter μ^+ has been transformed into an incoming wave controlled now by the parameter μ^-. Actually, the probability for a return is amplified by the fact that the force constant for contraction is larger than that for expansion, in terms of parameters $\mu^+ > |\mu^-|$. This incoming wave plays now the same role as the initially incoming wave described in "Step 1". In consequence of that a chain reaction

can travel along a whole chain of atoms; *i.e.* a current has been transported along the chain.

4. Final Remarks

At a first glance, a super current triggered off alone by correlation may surprise. However, other surprising dominant correlation effects in few-electron atoms are known, see for instance [12]. Finally, we stress that this current does not suffer in any of the three steps from inelastic collisions since the electron transport occurred by electron wave diffraction rather than by particle transportation accompanied by collisions.

Acknowledgements

The author acknowledges gratefully financial support provided by DFG during the initial stages of correlation studies.

Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

References

[1] Hunklinger, S. (2018) Festkörperphysik. De Gruyter, Heidelberg. https://doi.org/10.1515/9783110567755

[2] Bardeen, J., Cooper, L.N. and Schriefer, J.R. (1957) Theory of Superconductivity. *Physical Review*, **108**, 1175. https://doi.org/10.1103/PhysRev.108.1175

[3] Little, W.A. (1968) Superconductivity at Room Temperature. *Scientific American*, **212**, 21. https://doi.org/10.1038/scientificamerican0265-21

[4] Pickelt, W.E. (1965) Superconductivity in Pure La and LaGd. *Scientific American*, **212**, 31.

[5] Antonovic, A. (1974) Prediction of Ambient-Pressure Superconductivity in Ternary Hybrid PdC. *Nature*, **247**, 358. https://doi.org/10.1038/247358a0

[6] Wannier, G. (1957) Threshold Ionization of H Atoms by Electrons. *Physical Review*, **90**, 817. https://doi.org/10.1103/PhysRev.90.817

[7] Klar, H.J. (2020) The Born-Oppenheimer Approximation Revisited. *JAMP*, **8**, 2416. https://doi.org/10.4236/jamp.2020.811178

[8] Macek, J.H. (1964) Properties of Autoinoning Staes of He. *Journal of Physics B*, **1**, 811.

[9] Klar, M. and Klar, H. (1980) Accurate Calculation of Doubly Excited States of Two-Electron Atoms Using Hyperspherical Coordinates. *Journal of Physics B*, **13**, 1057. https://doi.org/10.1088/0022-3700/13/6/014

[10] Fano, U. (1976) priv. comm.

[11] Klar, H. (2020) The Banach Space of Multiply Excited Atoms. *JAMP*, **8**, 1507. https://doi.org/10.4236/jamp.2020.88116

[12] Klar, H. (2020) Dominant Correlation Effects in Two-Electron Atoms. *JAMP*, **9**, 3230. https://doi.org/10.4236/jamp.2021.912211

Appendix

It is the purpose of this Appendix to show that the evolution given by (18) solves initial value problems of the parabolic Equation (17).

The initial value is in our case provided by the separated system with one electron in a Rydberg orbital.

The other one is fare away, *i.e.* $R=\infty$. To this end we investigate the quantity

$$N=\lim_{R\to\infty}\int_{-\pi/4}^{+\pi/4}\mathrm{d}\beta\, T(\beta)\exp\left\{i\mu\sqrt{R}\left(\beta-\beta'\right)^2\right\} \tag{A1}$$

Since the exponential oscillates rapidly for $R\to\infty$ we extend the integration interval to $-\infty<\beta<+\infty$, and substitute $i\mu\sqrt{R}\left(\beta-\beta'\right)^2=x^2$. Thus we obtain

$$N=T(0)\sqrt{\frac{\pi}{\mu}}R^{-\frac{1}{4}}\mathrm{e}^{i\frac{\pi}{4}}\delta\left(\beta-\beta'\right) \tag{A2}$$

In the last step we have used

$$\int_0^{+\infty}\exp\left\{-x^2\right\}\mathrm{d}x=\sqrt{\pi}\,. \tag{A3}$$

Thus we have proven that the Fresnel distribution (18), converges to a delta distribution provided $\mu>0$. Therefore we have identified the Fresnel distribution for $\mu>0$ to deliver the quantum analogue of Wannier's converging trajectory.

In contrast to that we remark that the expression A1 diverges for $\mu<0$. That is easily seen if we proceed as above we would end with the diverging integral

$$\int_0^{\infty}\mathrm{e}^{+x^2}\mathrm{d}x$$