

Abstract for Road to RTSC, Loen, Norway
17 June 2007

Does the Da Vinci Code Hold the Key to Room Temperature Superconductivity

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The year 1957 witnessed what might have been the most important theoretical advance in condensed matter physics of the past century. Bardeen, Cooper and Schreiffer¹ were able to show, based on an elegantly simple proof by Cooper that the degenerate Fermi gas could be gapped by weak lattice vibration-mediated attractive electron-electron interactions, that the transition temperature of superconductors could be semi-quantitatively given by the expression, $T_C = a\theta_D \exp(-1/\lambda)$. Here T_C is the critical temperature, θ_D the phonon Debye temperature, λ the dimensionless electron phonon coupling constant, and a a “gap scaling factor” of order 1-3. Strictly speaking, this simple “BCS relation” holds only for $\lambda < 1$, and $\lambda k\theta_D \ll E_F$, where E_F is the Fermi energy. However, Migdal and Eliashberg² later showed modifications of this relation that included higher order attraction terms as well as electron-electron repulsion could accommodate “strong coupling” values of λ in the range 1 – 2 and thus successfully account for the relatively high transition temperatures of the A15 compounds and perhaps the HTSC cuprates as well. The message of BCS is clear: a superfluid state is mediated by the pairing of fermions in a boson field, and its condensation temperature scales both with the characteristic temperature of the boson and the strength of its coupling to the fermions. It is possible that attempts to increase T_C by engineering a rise in the electron-phonon λ , given the known range of Debye temperatures available, may give rise to unphysical material constraints.³ Even other possible “boson flavors,” e.g., “magnons or “spin waves” or “resonating bonds,” may not possess characteristic energies large enough to get T_C to room temperature with realistically achievable coupling constants. On the other hand, various sorts of charge polarization bosons, such as excitons, have characteristic energies on the order of 1 eV and in principle could manifest in properly designed structures superconducting transition temperatures on the order of 300 K, even under extremely weak electron-exciton coupling. This opportunity did not go unnoticed and was suggested (before BCS!) by Fritz London⁴ as possible in macro-organic molecules, and analytically addressed post-BCS by Davis, Gutfreund and Little,⁵ Ginzburg,⁶ and Allender, Bray and Bardeen,⁷ and was even the subject of a science fiction short story in 1998.⁸

In this lecture, we will review the several model approaches taken in the past in light of their possible incorporation in modern density functional theory employing today’s powerful and widely available computational hardware and software applied to novel structures now accessible by “nano-assembly” and “nano-machining” technologies. We will address one of the “devils in the details” of all such models, the required spatial separation of electron transport from the polarization portions of any hypothetical

material embodiment, which often contain quasi-one-dimensional metal chains subject to gapping of their Fermi through commensurate structural distortion. As the title of the lecture hints, there may exist in the wisdom of the ancients some rituals to exorcise this devil.

¹ J. Bardeen, L. N. Cooper and J. R. Schrieffer, Phys. Rev. 108, 1175 (1957).

² A. B. Migdal, Sov. Phys. JETP 5, 1174 (1958); G. M. Eliashberg, Sov. Phys. JETP 11, 1364 (1959).

³ M. R. Beasley – This conference

⁴ F. London, “Superfluids,” (John Wiley & Sons, London, 1950), pp. 8-9.

⁵ D. Davis, H. Gutfreund and W. A Little, Phys. Rev. B13, 4766 (1976).

⁶ V. L. Ginzburg, Sov. Phys. Usp. 13, 335 (1970).

⁷ D. Allender, J. Bray and J. Bardeen, Phys. Rev. B7, 1020 (1973).

⁸ P. M. Grant, Physics Today, May 1998.